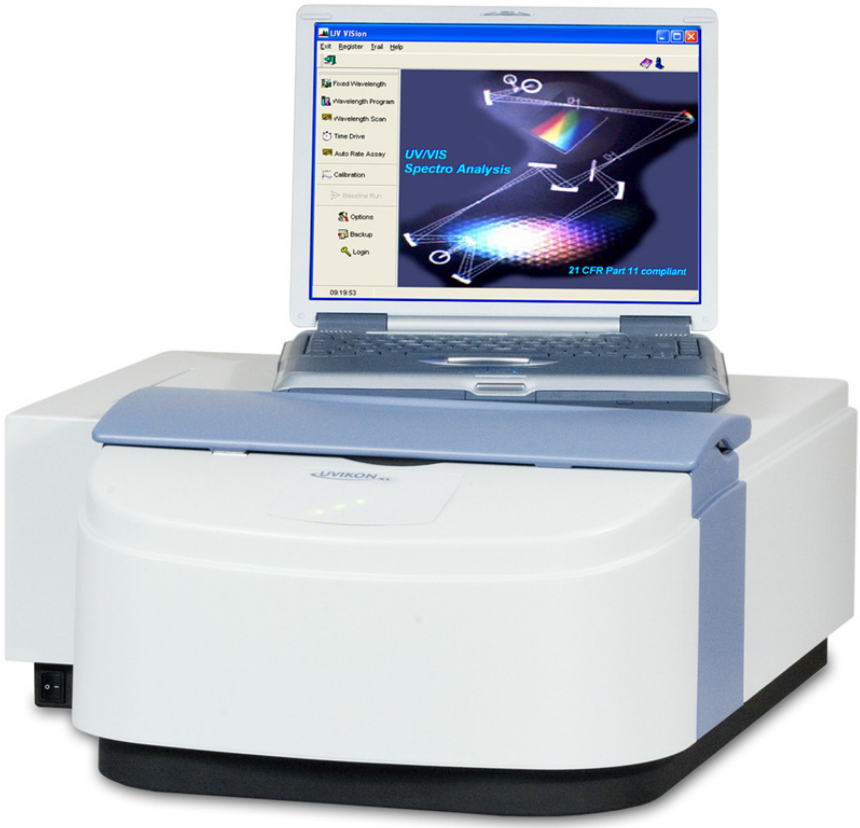
SOFTWARE USER MANUAL



UVS Software
for
UVIKON 900 / XL / XS

Table of Contents

1. GENERAL INFORMATION 9
1.1. GENERAL WARNINGS 9
1.2. CD CONTENT 9
1.3. INSTALLATION and REGISTRATION 9
2. OPERATING INSTRUCTIONS 10
2.1. INTRODUCTION 10
2.1.1. System Icons 10
2.2. SET-UP 12
2.2.1. Starting 12
2.2.2. Options 12
2.2.2.1. General options *13*
After changing com ports please start UVS again. *14*
2.2.2.2. Audit Trail *15*
2.2.2.3. Print Control options *16*
2.2.2.4. Extras *17*
2.2.2.5. Projects *18*
2.2.3. Backup 19
2.2.3.1. Backup *19*
2.2.3.2. Restoring Backup Data *19*
2.2.3.3. Archive *21*
2.2.4. User management 23
2.2.4.1. Password *24*
2.2.4.1.1. User rights *24*
2.2.4.1.2. Adding users *25*
2.2.4.1.3. Login rights *25*
2.2.4.1.4. Login blocked *25*
2.2.4.1.5. Additional Rights *25*
2.2.4.1.6. Saving data *25*
2.2.4.1.7. Password expired *26*
2.2.4.1.8. Password *26*
2.2.4.2. Groups *26*
2.2.5. Baseline 27
2.2.6. Power on 28
2.2.7. Self test and system software initialisation 28
2.2.8. Exiting the system software 29
2.3. OPERATION 29
2.3.1. General guidelines 29

2.3.1.1. Acquisition-Calculate-Display 29
2.3.1.2. Recommended Operating Practise 29
2.3.1.3. The Acquisition Window 30
2.3.1.4. The Method Window 32
2.3.1.5. The Report Window 32
2.3.1.6. Quick Search Function and Row Colouring 33
2.3.2. Starting a measurement 34
2.3.3. Recalculation 34
2.3.4. Saving data 35
2.3.5. Loading existing data files 35
2.3.6. Data conversion to EXCEL format 36
2.3.7. Export to Clipboard 36
2.3.8. ASCII Export 36
2.3.9. Methods 36
2.3.10. Saving methods 38
2.3.11. Cancel all current activities 38
2.3.12. Activate Cursor and Manual Peak Picking 38
2.3.13. Zooming 39
2.3.14. Adding comments to curves 40
2.4. SYSTEM MODES 41
2.4.1. Fixed Wavelength 41
2.4.1.1. The Acquisition Screen in Fixed Wavelength 41
2.4.1.1.1. Statistic 42
2.4.1.1.2. Instrument Control 42
2.4.1.1.3. Run parameters 42
2.4.1.1.4. System Status 44
2.4.1.2. Parameters in Fixed Wavelength Acquisition 44
2.4.1.3. The Method in Fixed Wavelength 45
2.4.1.3.1. Acquisition parameters 45
2.4.1.3.2. Common Parameters 46
2.4.1.3.3. Calculation 47
2.4.1.3.4. Concentration 48
2.4.1.3.5. Audit Trail in Fixed Wavelength Method 48
2.4.1.4. The Report Screen in Fixed Wavelength 48
2.4.1.4.1. Printing 49
2.4.1.4.2. Importing a report from the database 49
2.4.1.4.3. Filtering the report list 49
2.4.1.4.4. Audit Trail in Fixed Wavelength Report 50
2.4.1.5. Calculations in Fixed Wavelength 50
2.4.1.6. Concentration in Fixed Wavelength 51
2.4.2. Wavelength Scan 51
2.4.2.1. The Acquisition Screen in Wavelength Scan 51
2.4.2.1.1. Run parameters 52
2.4.2.1.2. System Status 53
2.4.2.2. The Method in Wavelength Scan 53

2.4.2.2.1. Acquisition parameters 54
2.4.2.2.2. Common Parameters 55
2.4.2.2.3. Calculation 55
2.4.2.2.4. Curve Parameters in the Wavelength Scan Method 55
2.4.2.2.5. Calculation Parameters in the Wavelength Scan Method 56
2.4.2.2.6. Audit Trail in Wavelength Scan Method 57
2.4.2.3. The Report Screens in Wavelength Scan 57
2.4.2.3.1. The "Overview" Report Screen 57
2.4.2.3.2. Printing 58
2.4.2.3.3. Importing a report from the database 58
2.4.2.3.4. Filtering the report list 59
2.4.2.3.5. The "Chart" Report Screen 59
2.4.2.3.6. "Chart" Report Screen Functions 60
2.4.2.3.7. Audit Trail in Wavelength Scan Report 61
2.4.2.4. Calculations in Wavelength Scan 61
2.4.2.5. Peak Detection 62
2.4.2.6. Overlay 63
2.4.2.7. Joined Reports 65
2.4.2.8. Wavelength Scan Measurement Example 67
2.4.3. Time Drive 69
2.4.3.1. The Acquisition Screen in Time Drive 69
2.4.3.1.1. Run parameters 69
2.4.3.1.2. System Status 70
2.4.3.2. The Method in Time Drive 71
2.4.3.2.1. Acquisition parameters 72
2.4.3.2.2. Common Parameters 72
2.4.3.2.3. Calculation 72
2.4.3.2.4. Curve Parameters in the Time Drive Method 73
2.4.3.2.5. Calculation Parameters in the Time Drive Method 73
2.4.3.3. The Report Screens in Time Drive 74
2.4.3.3.1. The "Overview" Report Screen 74
2.4.3.3.2. Printing 74
2.4.3.3.3. Importing a report from the database 75
2.4.3.3.4. Filtering the report list 75
2.4.3.3.5. The "Chart" Report Screen 76
2.4.3.3.6. "Chart" Report Screen Functions 76
2.4.3.4. Calculations in Time Drive 77
2.4.3.5. Time Drive Measurement Example 78
2.4.4. Auto Rate Assay 81
2.4.4.1. The Acquisition Screen in Autorate Assay 81
2.4.4.1.1. Run parameters 82
2.4.4.1.2. System Status 83
2.4.4.2. The Method in Autorate Assay 83
2.4.4.2.1. Acquisition parameters 84
2.4.4.2.2. Common Parameters 84
2.4.4.2.3. Calculation 85
2.4.4.2.4. Wavelength 85
2.4.4.2.5. Curve Parameters in the Auto Rate Assay Method 85

2.4.4.2.6. Calculation Parameters in the Auto Rate Assay Method 86
2.4.4.3. The Report Screens in Autorate Assay 87
2.4.4.3.1. The "Overview" Report Screen 87
2.4.4.3.2. Printing 87
2.4.4.3.3. Importing a report from the database 88
2.4.4.3.4. Filtering the report list 88
2.4.4.3.5. The "Chart" Report Screen 89
2.4.4.3.6. "Chart" Report Screen Functions 89
2.4.4.4. Calculations in Autorate Assay 90
2.4.5. Wavelength Program 92
2.4.5.1. The Acquisition Screen in Wavelength Program 92
2.4.5.1.1. Run parameters 93
2.4.5.1.2. System Status 94
2.4.5.2. The Method in Wavelength Program 94
2.4.5.2.1. Acquisition parameters 95
2.4.5.2.2. Common parameters 95
2.4.5.2.3. Wavelength Program calculations 96
2.4.5.2.4. Calculation 97
2.4.5.2.5. Audit Trail in Wavelength Program Method 97
2.4.5.3. The Report Screen in Wavelength Program 97
2.4.5.3.1. Printing 98
2.4.5.3.2. Importing a report from the database 98
2.4.5.3.3. Filtering the report list 98
2.4.5.3.4. Audit Trail in Wavelength Program Report 99
2.4.5.4. Calculations in Wavelength Program 99
2.4.5.5. Wavelength Program Measurement Example 100
2.5. CALCULATIONS 104
2.5.1. Curve Functions 104
2.5.1.1. Derivative 105
2.5.1.2. Show cross-points 105
2.5.1.3. Smoothing 105
2.5.1.4. Calculation 106
2.5.1.5. Peak Detection 106
2.5.2. Activity 107
2.5.2.1. Activity Results 111
2.5.3. Concentration Factor 111
2.5.4. Wavelength Program functions 111
2.5.5. Linear Calibration 111
2.5.5.1. Creating a Calibration File 111
2.5.5.2. Using a Calibration Curve 115
2.5.6. Quadratic Calibration 117
2.6. REPORTING 118
2.6.1. Printing 118
2.7. REPORT MANAGER 121

2.7.1. Templates 122
2.7.1.1.1. How to print single curves in the applications Scan, Timedrive, Auto Rate Assay 125
2.7.1.2. Create and select templates and template blocks 126
2.7.1.3. List of some predefined report templates 131
2.8. Report design editor 132
2.8.1. Controls 133
2.8.1.1. Key control 133
2.8.1.2. Mouse control 133
2.8.2. Toolbars 134
2.8.2.1. Designer mode bar 134
2.8.2.2. "Standard" toolbar 134
2.8.2.3. "Text" toolbar 135
2.8.2.4. "Frame" toolbar 136
2.8.3. "Align" toolbar 136
2.8.4. Designer options 137
2.8.5. Report settings 139
2.8.6. Page options 141
2.8.7. Creating reports 143
2.8.7.1. Report objects 143
2.8.7.2. "Hello, World!" report example 144
2.8.8. The "Text" object 144
2.8.9. HTML-tags in the "Text" object 146
2.8.10. Displaying expressions with the help of the "Text" object 147
2.8.11. Bands in Report Designer 148
2.8.12. "Picture" object 150
2.8.13. Chart object 151
2.8.14. Stringgrid object 151
2.8.15. Data splitting 152
2.8.16. Child-bands 154
2.8.17. Shifting objects 155
2.8.18. Headers and footers of a data band 156
2.8.19. Report viewing, printing and export 158
2.8.20. Control keys 159
2.8.21. Mouse control 160
2.8.22. Report printing 160
2.8.23. Text search in report 162
2.8.24. Report Export 163
2.8.25. Export to PDF Format 163
2.8.26. Export to RTF Format 164
2.8.27. Export to Excel 165
2.8.28. Export to XML Format 166
2.8.29. Export to CSV Format 167

2.8.30. Export into HTML Format 168
2.8.31. Export to Text Format 169
2.8.32. Report Design References 170

2.9. Managing curves 174
2.9.1. Direct Printing of Curves 174
2.9.2. Editing and Formatting of Charts 175
2.9.2.1. Changing the scaling (Axis) 175
2.9.2.1.1. Scales 176
2.9.2.1.2. Decimal Format 176
2.9.2.1.3. Title 177
2.9.2.2. Titles 177
2.9.2.3. Legend 177
2.9.2.3.1. Style 178
2.9.3. Audit Trail 178
2.9.3.1. Report Trail 179
2.9.3.2. Deleted Reports 179
2.9.4. Electronic Signature 179
2.9.4.1. Signing a Report 179
2.9.4.2. Signature Status Indications 182
2.9.4.2.1. Quick Overview 182
2.9.4.2.2. Detail Overview 182
2.9.4.2.3. Signature Audit Trail 183
2.9.4.3. Deleting a Signed Report 183

3. OPTIONS AND ACCESSORIES 184

3.1. AUTOMATIC CELL CHANGER 184
3.1.1. Installation 184
3.1.2. Cell Changer Mode (only UVSX) 184
3.1.2.1. 6 samples / 1 reference. 185
3.1.2.2. 6 samples / 6 references. 186
3.1.2.3. 10 samples / 2 references. 187
3.1.2.4. Manual operation (only UVSX) 188
3.1.3. Cell Changer operation in the different system methods 188
3.1.3.1. Auto rate assay 188
3.1.3.2. Fixed Wavelength 188
3.1.3.3. Wavelength Scan 188
3.1.3.4. Time Drive 188
3.1.3.5. Wavelength Program 188

3.2. Thermosystem / Thermopack 190
3.2.1. Installation 190
3.2.1.1. Manual operation 190

3.3. Stirrer (only UVSX) 190
3.3.1. Installation 190

3.4. Sipper 191
3.5. Liquid handler 193
3.6. Katalase 200

1. GENERAL INFORMATION

The user should be, before using the instrument, have read and understood this operating manual, particularly the general warnings given below.

1.1. GENERAL WARNINGS

- *Always disconnect the mains plug before starting any work inside the instrument*
- *Any maintenance operation inside the instrument, including lamp replacement, must be carried out by a service engineer or an authorized person. The user is normally only permitted access to the inside of the sample compartment.*
- *Keep the sample compartment clean*
- *Set wavelength to zero during transport to protect the drive mechanism*

1.2. CD CONTENT

The CD ROM supplied includes :

UVS Spectroscopy Software	Installation program
UVS User Manual	Software User Manual in pdf format
Adobe Acrobat Reader	Installation programs
UVS Software	Validation Certificate

1.3. INSTALLATION and REGISTRATION

The installation and registration procedures are described in a separate document. For the sake of completeness the login and setup procedures are also described in this document.

2. OPERATING INSTRUCTIONS

2.1. INTRODUCTION

This section of the manual describes the various operating possibilities available using the UVIKON. Please note that in all cases it is necessary to follow the general guidelines laid down in section 2.3 dealing with general operation. Examples give a step-by-step introduction to all system methods and calculation modes.

2.1.1. System Icons

The UVS software allows direct selection of many functions via a direct click on the corresponding icon. Many of these icons have the same function in different methods:

Saves the acquired data in the database. In addition, a report-file will be created in the corresponding directory for a given method. These report files can be viewed using the qrv.exe viewer.

Print preview and printing of a report.

Selection mask. You can select a view with date, method, user or name. The appropriate checkbox must be checked.

Transfers data to Excel. Data will be transferred directly to Excel. Excel must be installed for this function to be used. Note that this is not a file export and the data can then only be saved and processed within Excel.

Imports an earlier (extracted) database.

Opens an edit dialogue for reporting functions.

Exports a curve or table to the Windows clipboard for further processing.

Opens the calculation dialogue window or executes a re-calculation.

Opens the audit trail dialogue to allow viewing of the audit trail for a document

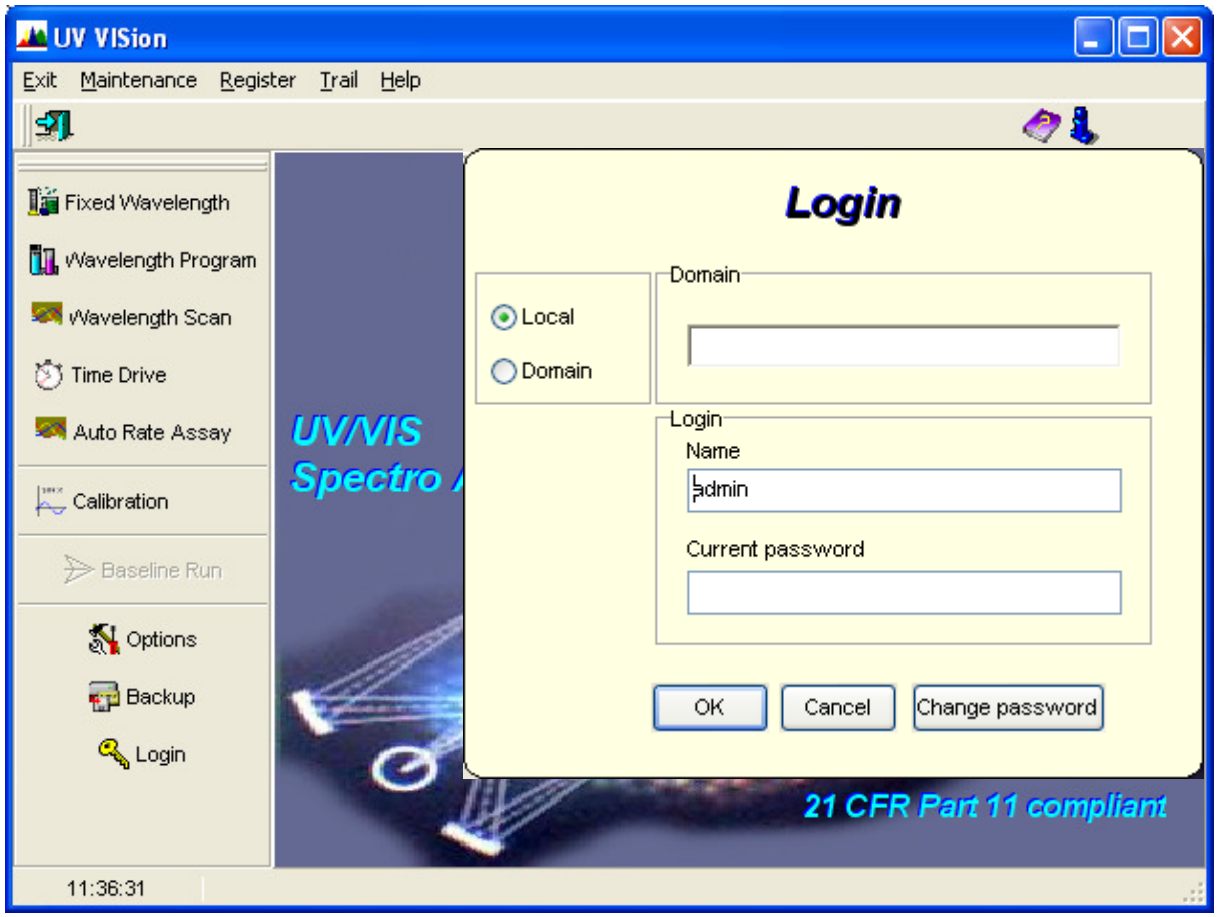
Opens the signature dialogue to allow signing of a document

Shows position of values on X- and Y-axis and allows to manually pick peaks and to add, edit or delete comments.

2.2. SET-UP

2.2.1. Starting

Ensure that the Uvikon is connected to the computer and is switched on. Then click on the UVS icon to start the software. The unit will first initialise, a prompt will appear for user name and password. User name and password are necessary because of the requirements of CFR Part 11 and permit only certain actions for users depending on the assigned permissions.

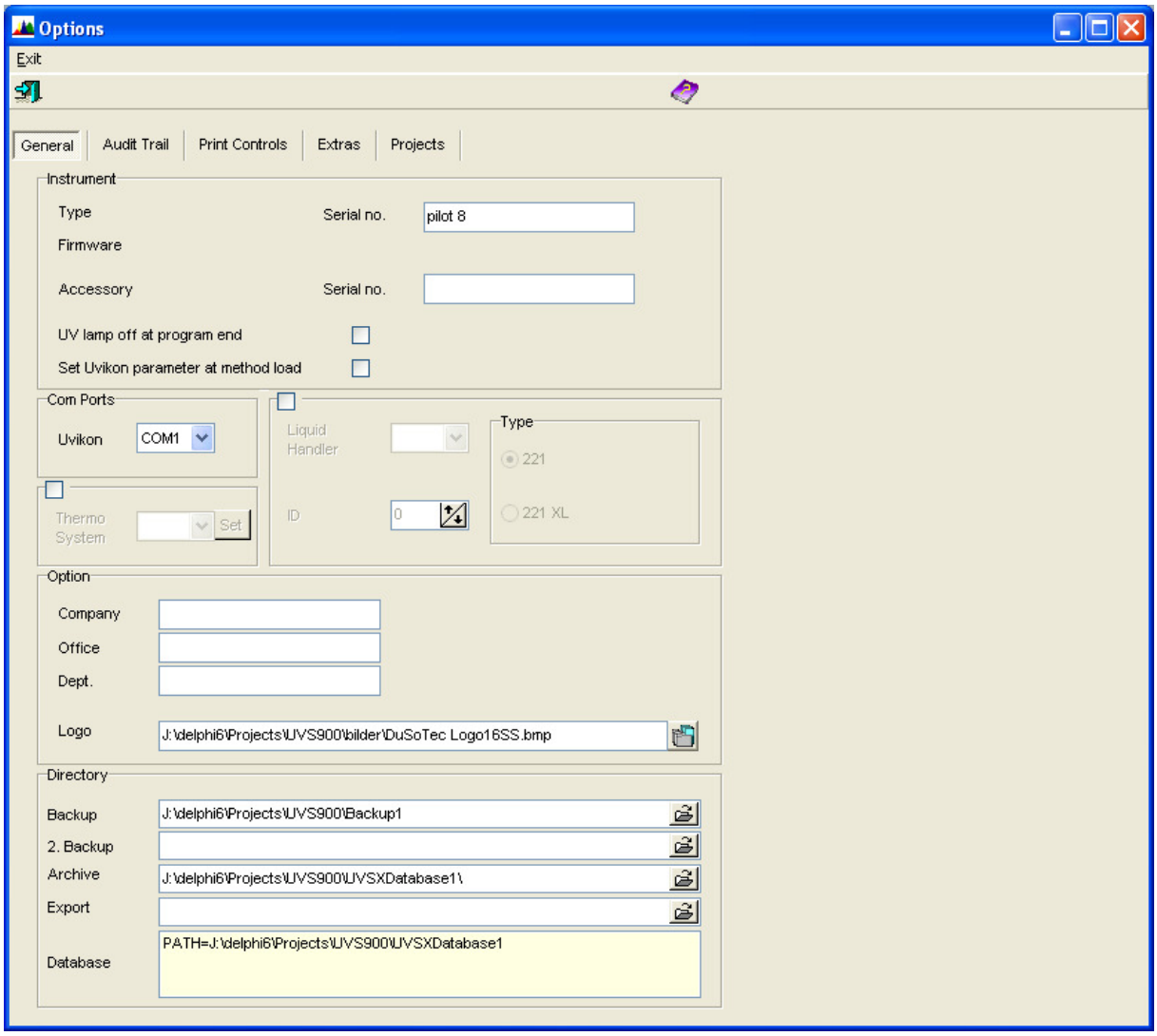


2.2.2. Options

Clicking on *Options* in the main display opens a dialogue window for entry of various parameters relating to reporting and archiving functions of the software.

2.2.2.1. General options

The first window is the “General” window for definition of company name etc. for inclusion on reports and also for the directory locations for the backup and database functions.



Instrument

The section contains data regarding the type of instrument, serial number and firmware used. In addition the accessories are listed and it is possible to enter also manually the serial number of the accessory.

UV lamp off …
If this box is checked the UV lamp will be switched off automatically at the end of the session.

Com Ports

Define the com ports for uvikon (only UVSX) and thermo system if needed, disable thermo system checkbox if no thermo system is connected.

After changing com ports please start UVS again.

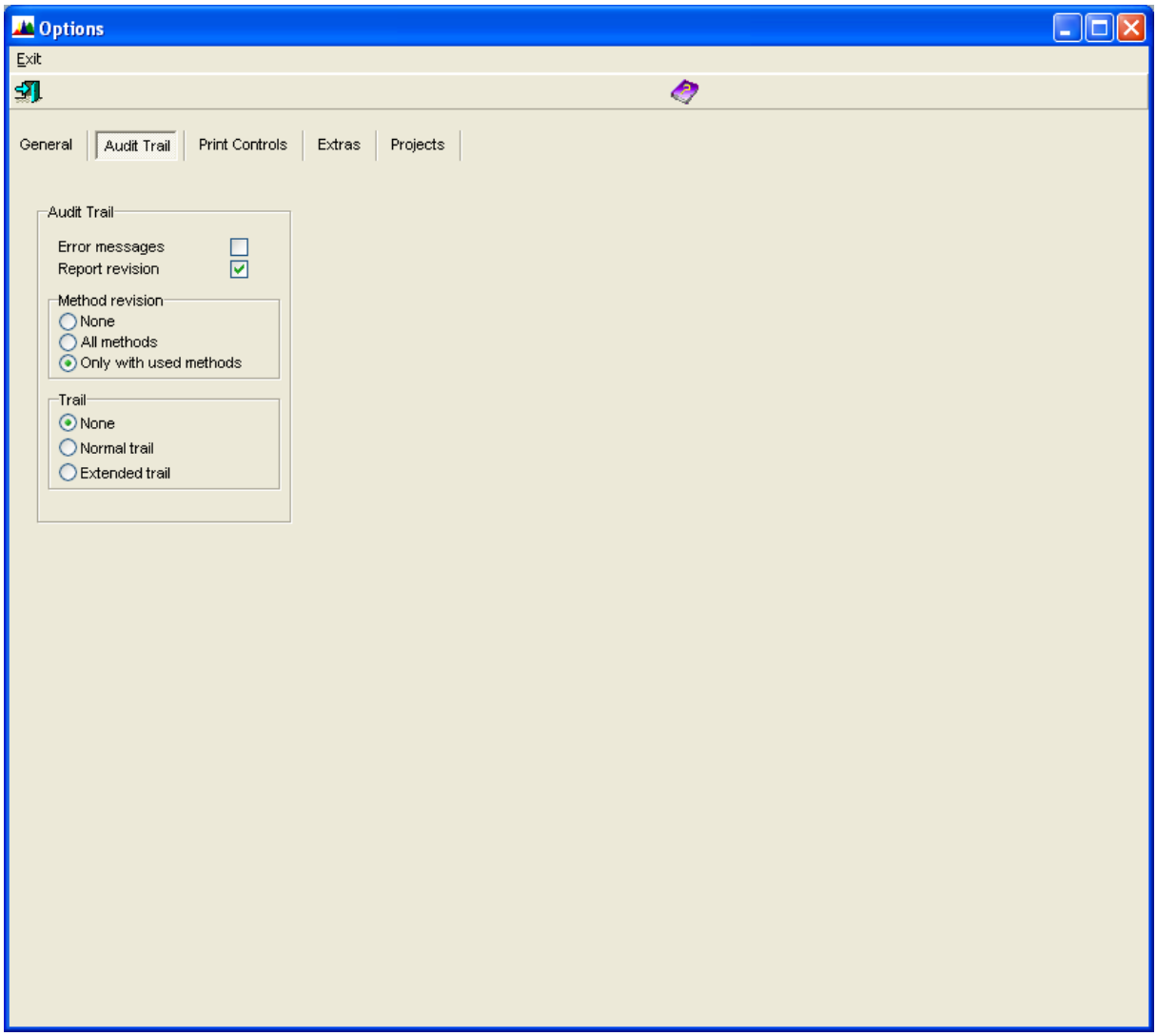
Options

These options define parameters which are included in the standard reports. Under Logo the location of a company logo file can be defined which is included in every printed report.

Directory

Here the location paths for the backup directories and database are defined. Definition of a second backup location is not necessary but recommended.

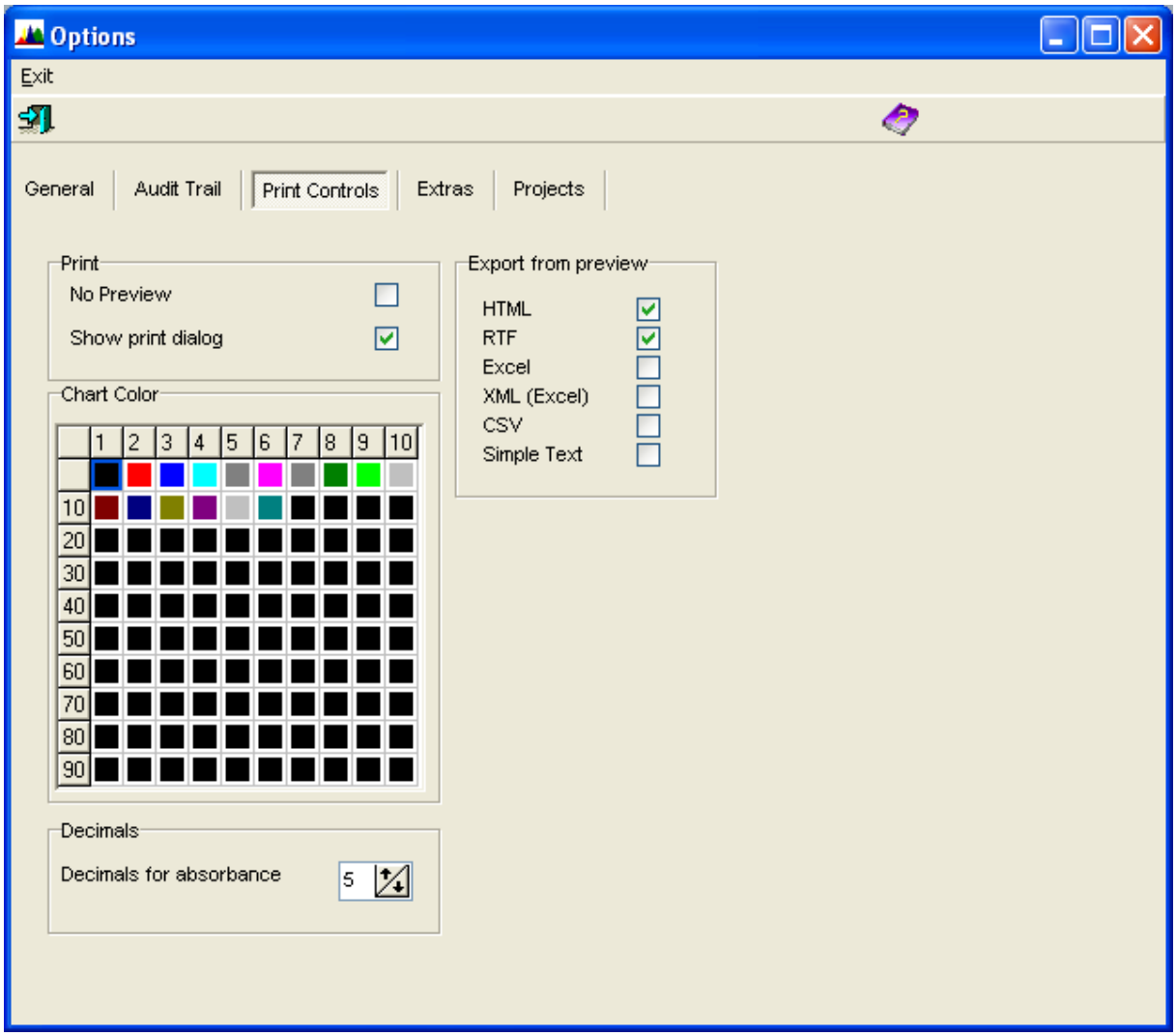
2.2.2.2. Audit Trail



Error messages	All displayed errors are stored in a text file if this option is checked.
Report revision	If this is checked a report cannot be changed. All modifications are saved in a copy of the original report and the revision index will be incremented.
Method revision	If this is checked a method cannot be changed. All modifications are saved in a copy of the original method and the revision index will be incremented.
Normal Trail	A trail is saved with the information user, time and what has changed.
Extended Trail	This is the normal trail with the additional information of old value and new value.

2.2.2.3. Print Control options

This window is accessed by clicking on the “Controls” tab and allows control of chart print format, chart colour, decimal points for diplayed absorbance values and audit trail.



Print Chart as Bitmap Normally the chart will be printed with vector graphic, but if your printer driver don’t print the graphic, try this option.

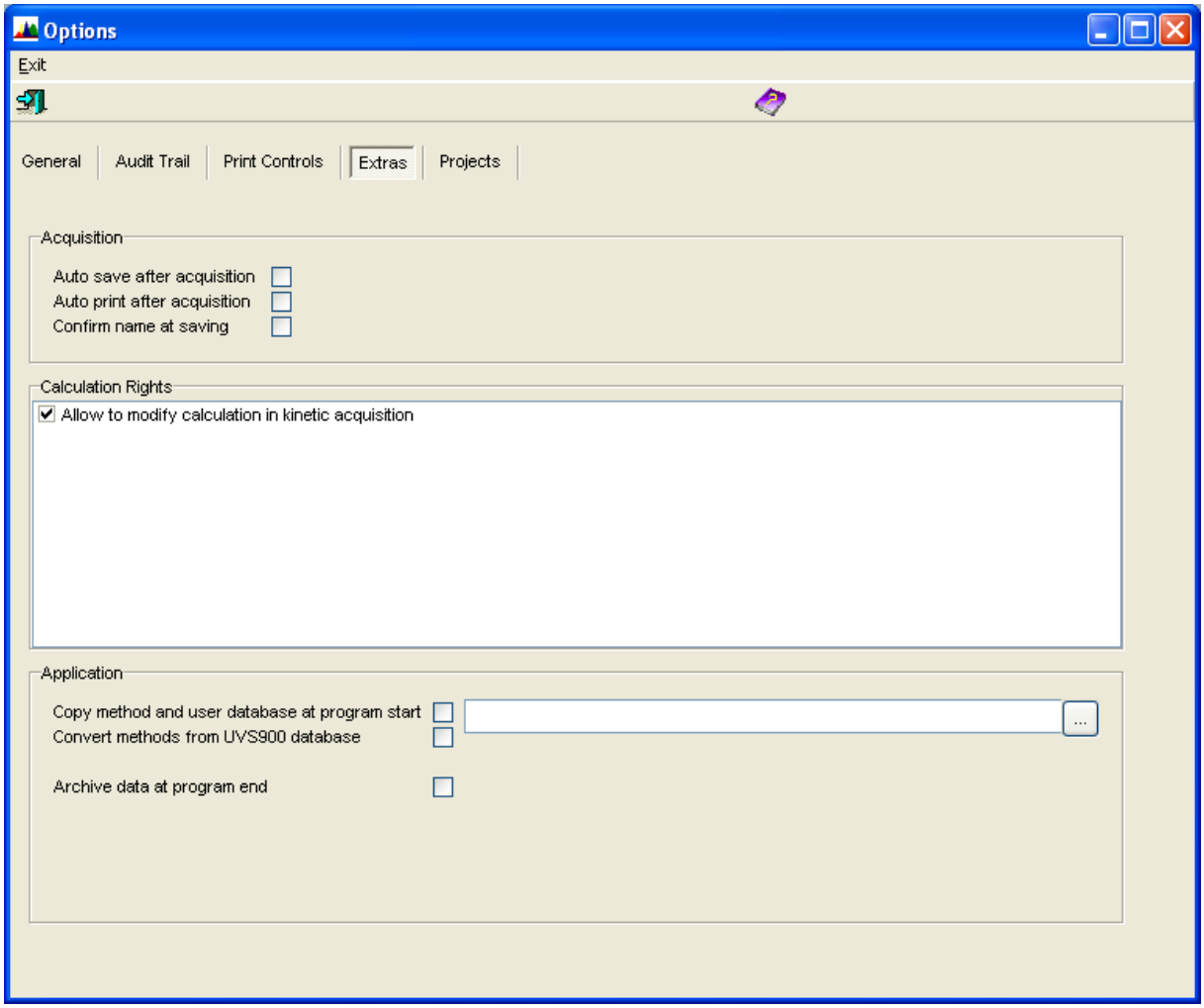
No Preview If you check this option the printout will be sent direct to the printer, otherwise the data is displayed with the preview on the screen.

Chart colour Colour table for curve colours in the order in which the curves are acquired. The colours may be selected individually.

Decimals for absorbance

Displayed and rounded values of the absorbance.

2.2.2.4. Extras

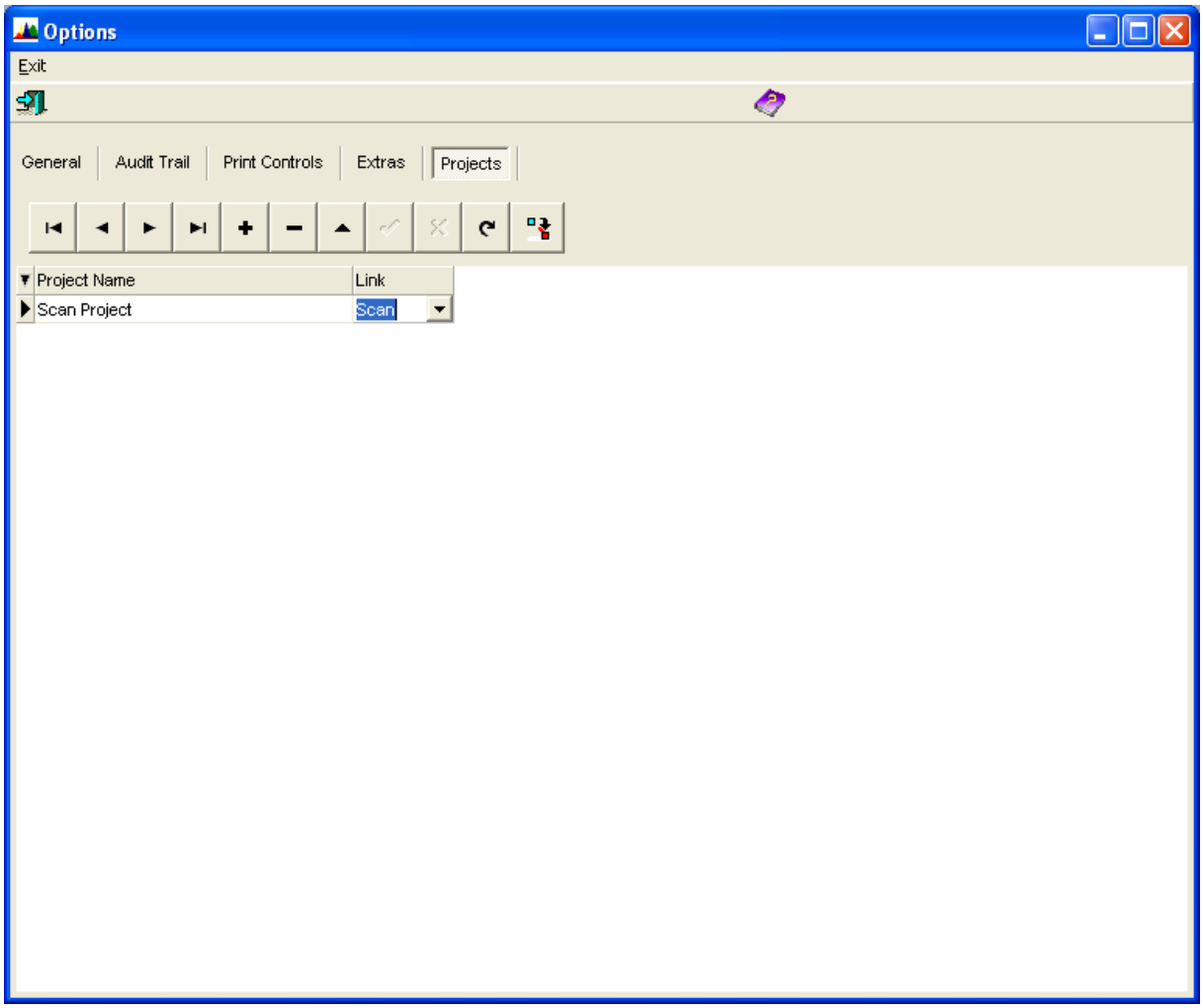


Autosave If this option is checked then the data will be saved automatically after acquisition.

Autoprint Please select for printing immediately after acquisition.

Note : See also the 'no preview option'

2.2.2.5. Projects

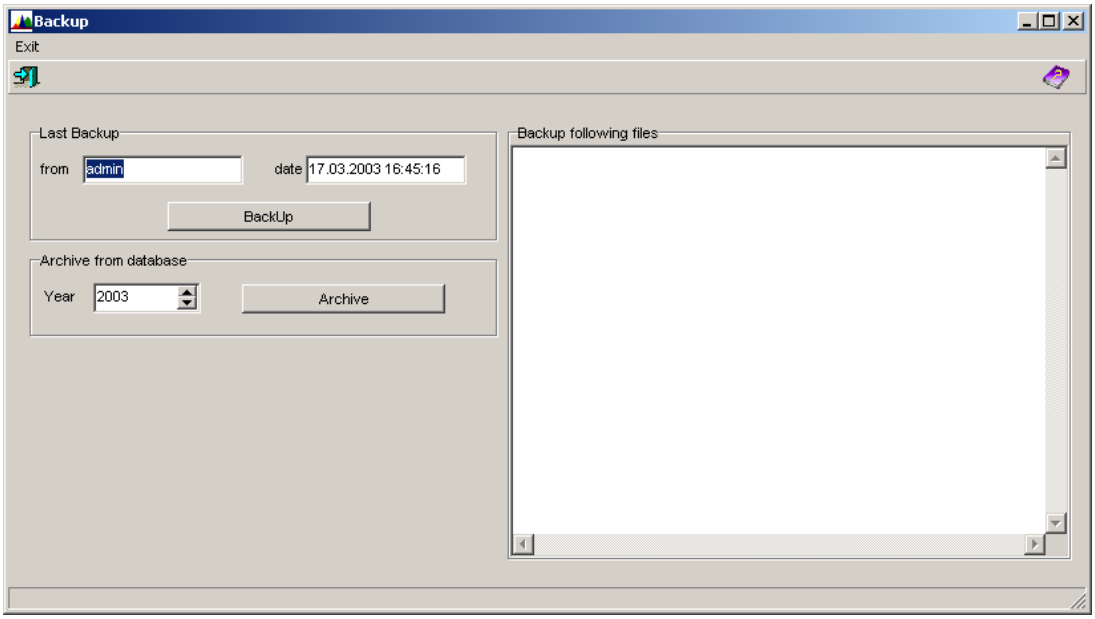


Define here your projects and link it with the methods (Fix wavelength, wavelength program, scan…)
The name of the project is saved with the report.

2.2.3. Backup

This function permits a backup or archive of either all data or an extract from the original database to a database sorted by year is possible.

The backup can be made to 2 independent servers via network, if the appropriate directory locations have been entered in the options section.



2.2.3.1. Backup

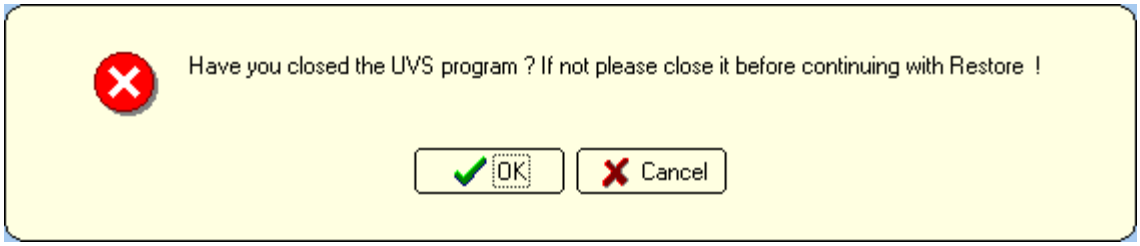
Clicking on the *Backup* button will execute a backup of the complete database to the directory locations defined in the Options menu. The right hand panel will display a listing of all files which will be backed up during the process. A confirmation dialogue is shown after successful execution of the backup:

The backup simply saves a copy of the working database files to the defined locations from which they can also be restored at any time as described below.

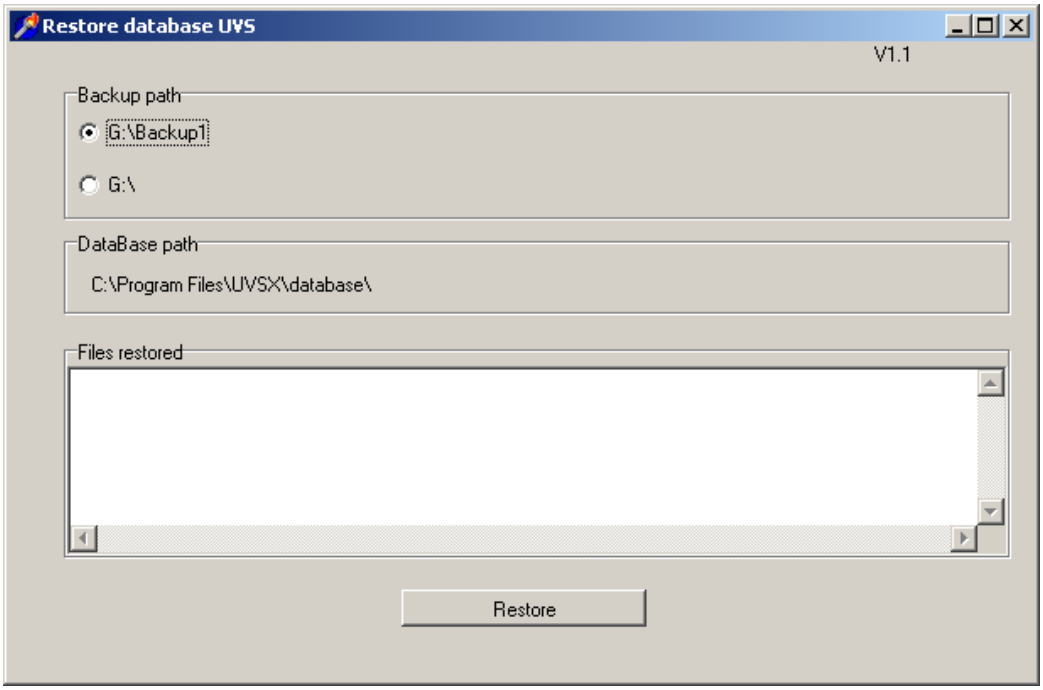
2.2.3.2. Restoring Backup Data

Restoring of previously backed up data is possible using the “restore UVS” application located in the UVS directory. In order to restore data you must close the normal UVS software before starting the restore process, a prompt will remind you of this before continuing:

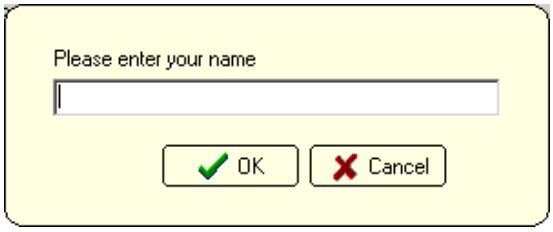
Start the restore UVS program, a prompt will appear to check that the main program has been closed:



Close if necessary and click on *OK* to obtain the restore dialogue:

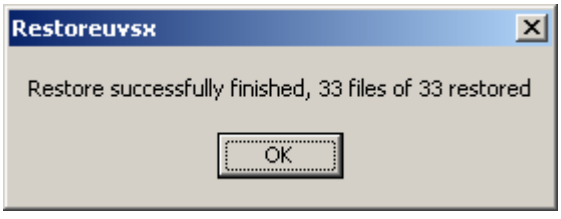


Specify the location from which you want to restore the data and click on the *Restore* button. You will be prompted to enter your name:



This name is required for record purposes and does not correspond with the user names installed for the main UVS software. Enter a name and click on *OK*.

The restore process will be confirmed:



2.2.3.3. Archive

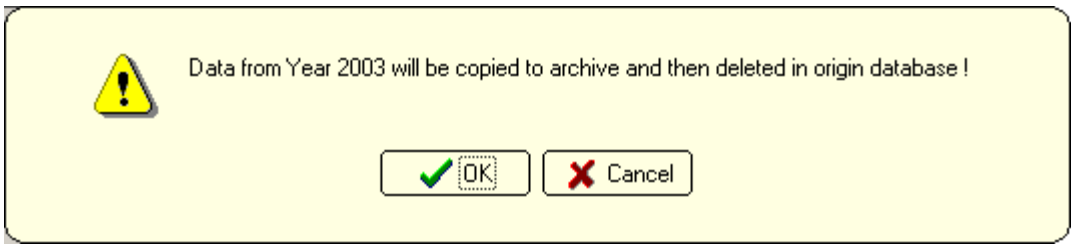
The archive is based on data obtained within any given year, e.g. all data collected during 2003. The data is then archived in the database and the original data removed locally.

Caution *It is possible to restore Archive data for viewing and modification during a working session. However, the restored data is automatically removed locally whenever Exit is executed. Modifications made during a session are automatically added to the archive data when exiting.*

The archive is not intended for storage of data which will be needed for comparison etc. Therefore, great care must be taken to select the ideal time to archive all data.

It is also possible to selectively control archiving by using the file based backup program module to save data before deleting that data in UVS which does not need to be archived immediately. The original data can then be restored as described above and the archived data removed.

The location of the archived database is pre-defined in the options page in the UVS software and therefore the user need only define the actual year to be archived and then click on the *Archive* button. A prompt appears requesting confirmation:



Click on *OK* to complete the archiving process.

1. Menu item: Options

↳ General Options

Setting the directories for Backup and Archive

Archive

Execution of Archiving in the Backup window of the main menu.

Prior to execution the year can be selected.

Backup

Execution of Backup in the Backup

Is saved with the Backup if a directory for the Archive was selected in the **`Database`** directory

Re-importing data from an Archive

Selection is made in the Report menu of a Method

- Selection of the year lists the corresponding data for the selected year
- Data can be re-calculated and partially combined (only within a given year)
- In the Report a range of search filters is available (Date, Text, etc.)
- The copying of data from one archive into another archive or the current data base is not possible.
- Users and Powerusers can also call up and re-process archived data, if the appropriate permissions in User Management have been set.

All files are saved in the **`Database`** directory.

(including sub-directories)

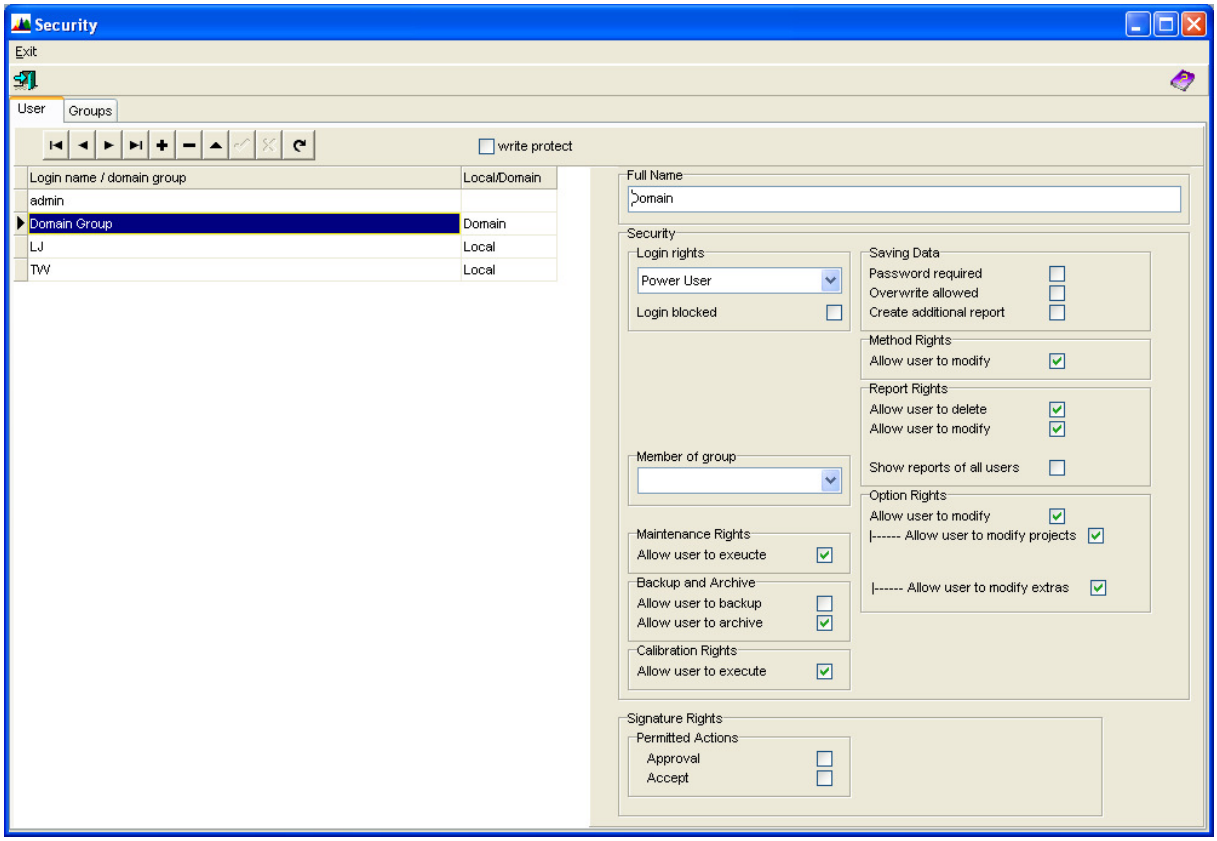
Two files are created:

`*.bck` File extension for the re-importing using the „Restore“ tool supplied

`*.zip` File extension for the manual re-import procedure using an „Unzip“ program, e.g. Winzip

2.2.4. User management

The UV Vision has its own login facility. A login name and a password is required to enter the program. The assignment of user rights, password administration etc is made by the administrator in a separate dialogue box accessed by clicking on the *Login* key in the main display.



2.2.4.1. **Password**

2.2.4.1.1. User rights

Generally three different user types are recognised with basic default permissions as described below:

	Action	Administrator	Power User	User
Main window	Fix Wavelength	yes	yes	yes
	Wavelength Program	yes	yes	yes
	Scan	yes	yes	yes
	Timedrive	yes	yes	yes
	Autorate Assay	yes	yes	yes
	Calibration	yes	Depends on security rights	
	Baseline Run	yes	yes	yes
	Option	Depends on security rights	Depends on security rights. Access only to print controls	Depends on security rights. Access only to print controls
	Backup	yes	Depends on security rights	
	Edit Security	yes	no	no
	Trail	yes	yes	yes
	Service	Depends on security rights		
Checked security rights	Password required on saving data	Depends on security rights		
	Overwrite existing report on saving data	Depends on security rights		
	Create additional report on saving data	Depends on security rights		
	Change Method	Depends on security rights		
	Delete Report	Depends on security rights		
	Modify Report	Depends on security rights		
	Signature approval	Depends on security rights		
	Signature accept	Depends on security rights		
Visibility	Report	all	Only own or grouped member reports	Only own or grouped member reports
	Method	all	all	all

The permissions for individual users are modified by the administrator by checking the appropriate boxes.

2.2.4.1.2. Adding users

In order to add a user it is always necessary to unclick the “write protect” checkbox and the click on the “+” or “-“ symbols to add or remove a user respectively.

Click on “+” and a dialogue box will prompt for a new user name:

Select local or domain and enter a name and click on *OK*, the new user will be entered in the list and the permissions for the new user can be selected using the dialogue boxes on the right of the window:

2.2.4.1.3. Login rights

Clicking on the drop-down arrow cause the three possible user types to be displayed as a drop-down list. Select the required user type from the list.

2.2.4.1.4. Login blocked

Clicking on this checkbox can be used to prevent a user from accessing the system temporarily. Permanent exclusion of a user should be made by deleting the user completely from the list using the “-“ button.

2.2.4.1.5. Additional Rights

Users can be assigned the right to delete reports. If this checkbox is not ticked the user is not allowed to delete reports.

2.2.4.1.6. Saving data

Clicking on the “Password required” checkbox will activate a password dialogue in order to permit saving of the acquired data. This security feature can be used to identify those users allowed to save data. Only the currently logged-in user provided with the appropriate rights can save data.

Clicking on the “Overwrite allowed” checkbox allows the user to also overwrite previously saved data.

Clicking on the “Create additional report” checkbox allows the user to save additional reports after creation of the initial report using the same acquired data.

2.2.4.1.7. Password expired

A change of password can be forced at certain intervals as defined by this dialogue. The option of never changing is also available but users should note that this option is not acceptable when operating in a controlled environment.

Entry of a time interval automatically produces a new box with the actual date by which the password must be changed.

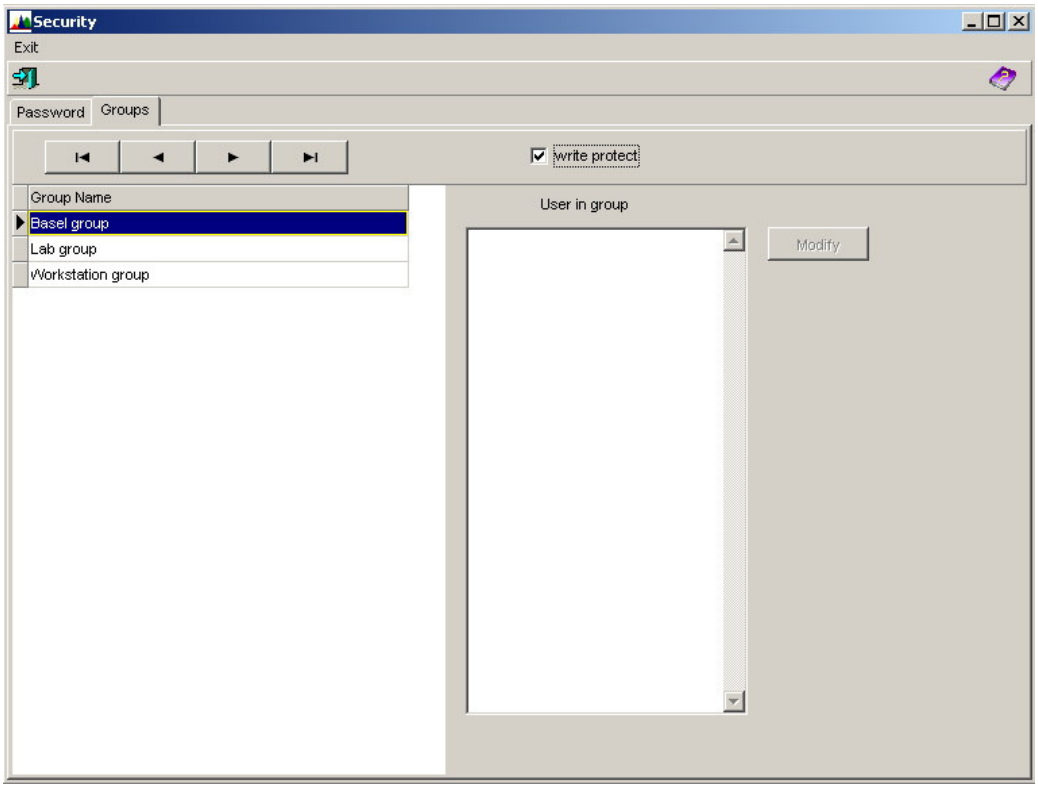
2.2.4.1.8. Password

This allows definition of the user password for normal access control and also for saving of data if the checkbox described is activated.

The initial password for the new user must be entered in the appropriate box. New users will be forced to change this password when they log onto the system for the first time. This is a precautionary measure to ensure that the system access password is known only to the user and no other third-party.

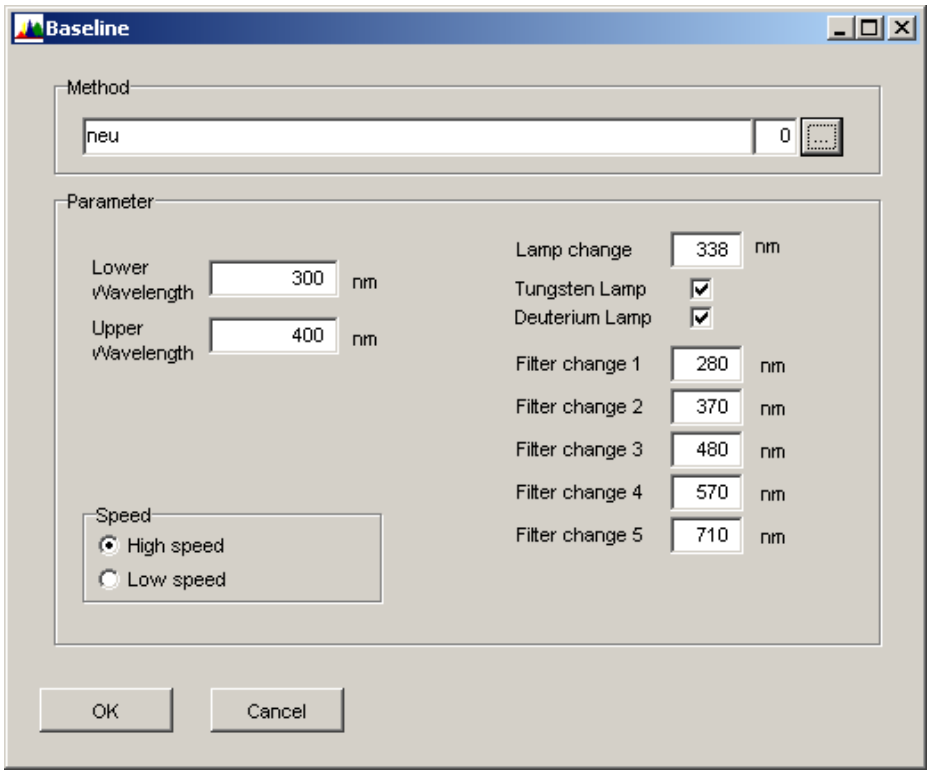
2.2.4.2. Groups

This defines the grouping for report access. Groups and members of groups can be defined to view the reports. A member of a group can view the reports of all members.



2.2.5. Baseline

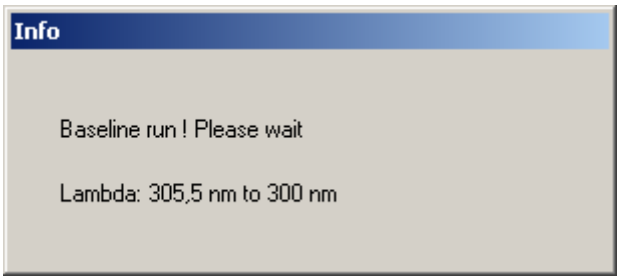
The UVS software does not automatically execute a baseline at start-up. This operation can be executed by clicking on the *Baseline Run* icon in the start-up screen to open the following dialogue window:



The actual conditions under which a baseline is executed can impact later measurement results if these are made using different parameters such as scan speed. For this reason the UVS software requires a method to be defined in *Wavelength Scan* mode before a baseline can be executed.

Click on the selection button adjacent to the method box in order to select the correct method if this is not already displayed. This method is then displayed before starting a baseline but can only be edited in the method editor itself thus permitting tracking of baseline conditions during normal operation.

Click on *OK* in order to start the baseline measurement, the unit will position itself at the correct starting wavelength and then automatically start the run:



2.2.6. Power on

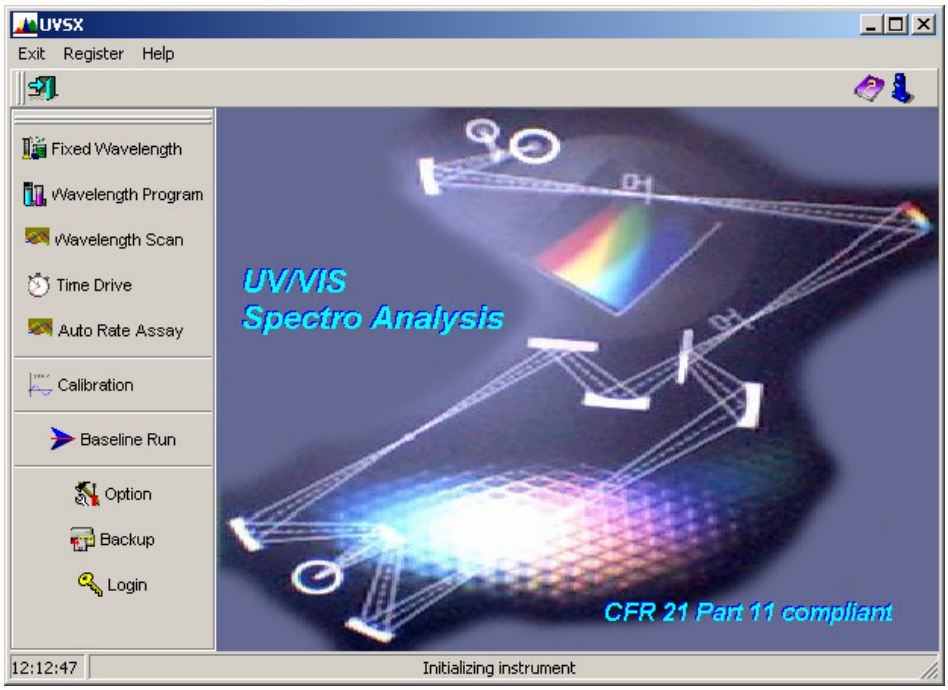
Switch on the power supply to the instrument, PC and monitor. The Uvikon has an indicator showing that the power is on. From the Windows Desktop click on the shortcut to display the start-up screen and login dialogue.

2.2.7. Self test and system software initialisation

The self test takes about 2 minutes (max) and performs the following checks:

- Program memory
- Data memory
- Tungsten halogen lamp on
- Deuterium lamp on
- Data transfer
- Wavelength drive

During self test you will see the main software window on the screen with "**Initializing instrument**" displayed on the bottom status bar.:



After completion of the initialisation this message will disappear and the software will prompt for user name and password for log in.

2.2.8. Exiting the system software

You can exit the system software by clicking either on the *Exit* icon in the top left corner or on the "**X**" in the top right corner.

2.3. OPERATION

2.3.1. General guidelines

2.3.1.1. Acquisition-Calculate-Display

The UVIKON uses an **A**cquisition-**C**alculate-**D**isplay scheme as shown below:

Acquire data for 1 to 10 samples using method parameters	➔	**C**alculate 1 to 10 samples using method parameters	➔	**D**isplay results of 1 to 10 samples using method parameters

The system is structured to use individual measurement modes, e.g. *Fixed Wavelength*, which must be pre-selected by the user. The selection of the mode to be used is made in the opening screen which can be accessed immediately after the software has started and login has been completed. This screen can also be reached at any time by exiting from the current mode in use.

2.3.1.2. Recommended Operating Practise

Each measuring mode uses *Acquisition* parameters which must be pre-defined in a *Method*. The *Method* also contains the data necessary for the final display of the results in the form of a *Report*.

The *Method* is the key to maintain a trace to all results and, together with the different reports, is subject to a strict revision control including an audit trail.

The method to be used can be selected from within the *Acquisition* page, where also the naming and number of samples to be analysed can be defined.

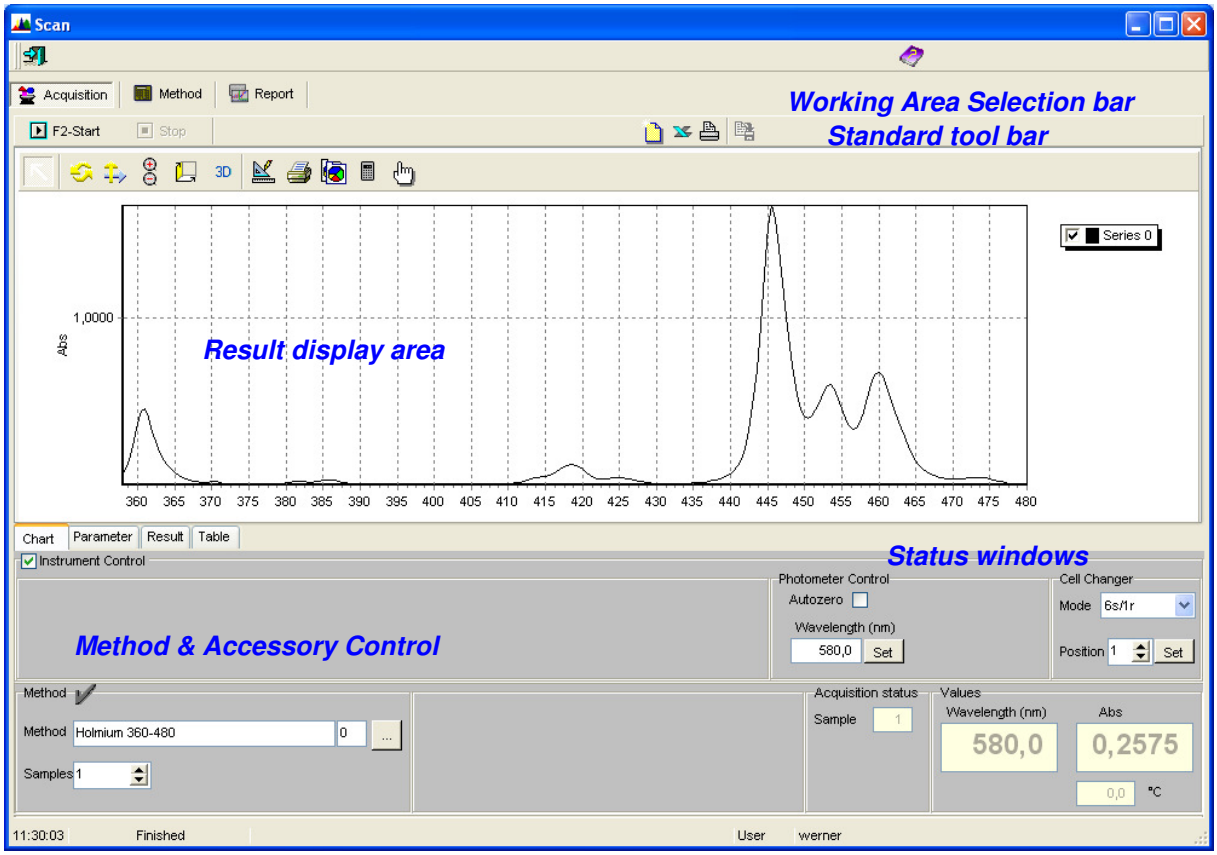
For routine testing the various *Methods* to be used will normally have been pre-defined and therefore it should not be necessary for users to access the *Method* screen. All necessary entries for simple routine operation with a series of samples can therefore be made directly in the *Acquisition* area.

A result report can also be previewed and printed directly from the *Acquisition* area and is therefore not necessary for the user to switch between the various main windows.

The individual windows for the three main operating areas are accessible via main buttons in the top section of each window and are described below:

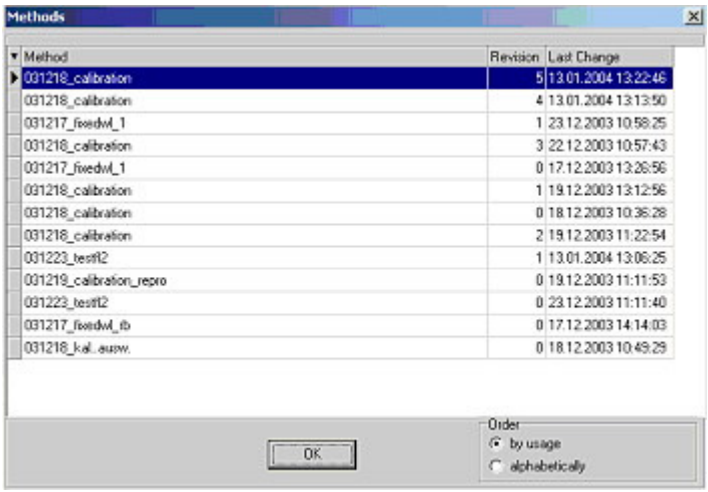
2.3.1.3. The Acquisition Window

The *Acquisition* page layout is similar for each mode and is shown below. A graphical display is only available for those measuring modes where graphics are actually required and used, e.g. *Wavelength Scanning*.

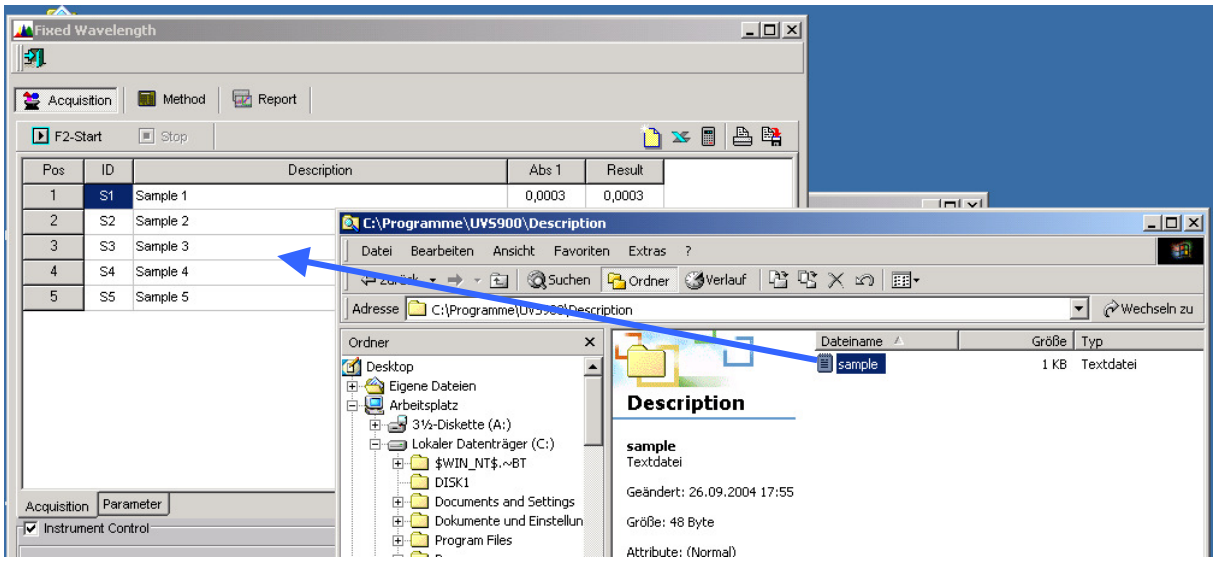


Working Area Selection	Buttons for selection of working window, e.g. *Method*.
Standard Toolbar	Contains buttons for starting and stopping measurements plus Excel export, printing and saving data for the currently open document.
Graphics Toolbar	Contains all functions required for controlling the appearance of the curve display, these are described in more detail below.
Status Windows	The status windows shows the current or last instrument status.
Method & Accessory Control	Enter the method name and the number of samples to be analysed.

The list for selecting methods may be sorted alphabetically or by the access counts. The most used method is on the top.

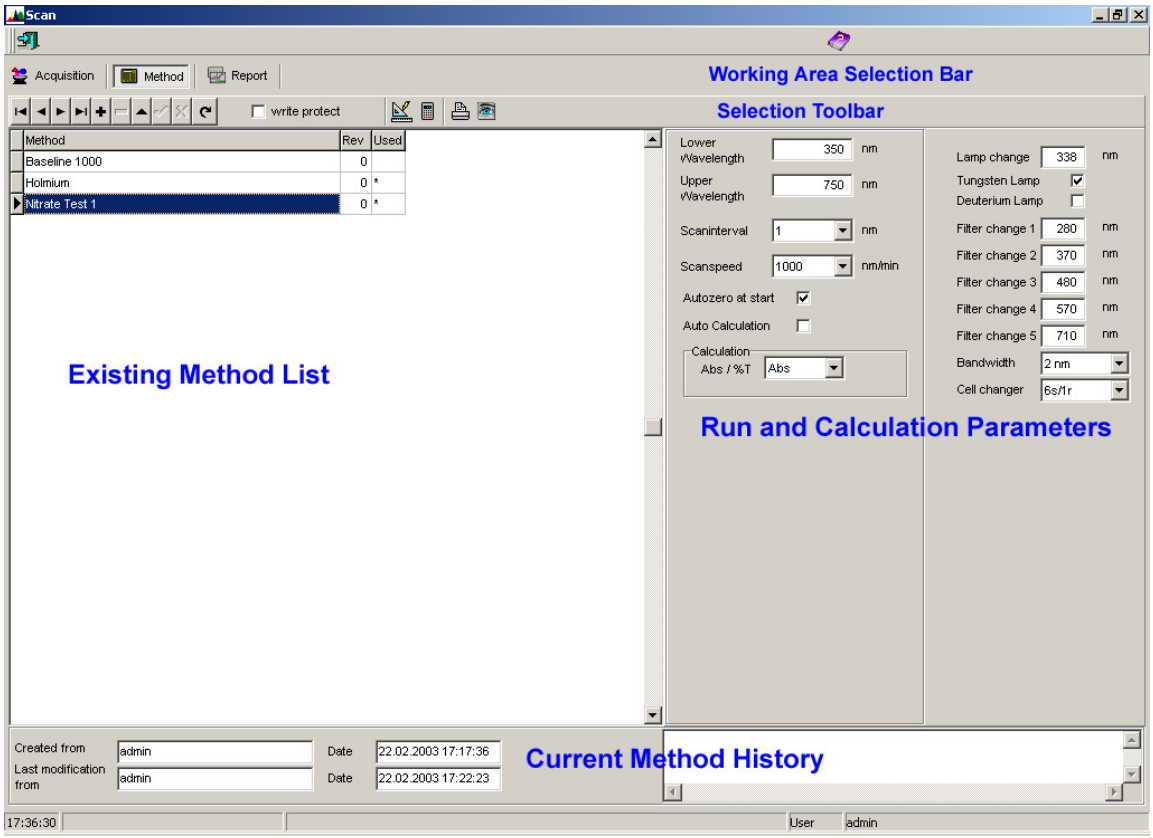


The sample description can be imported from a text file from the explorer via drag and drop.
Select the text file in the explorer and drag it with left mouse button pressed to the description grid.
Then release the mouse button, the text is dropped into the grid.



2.3.1.4. The Method Window

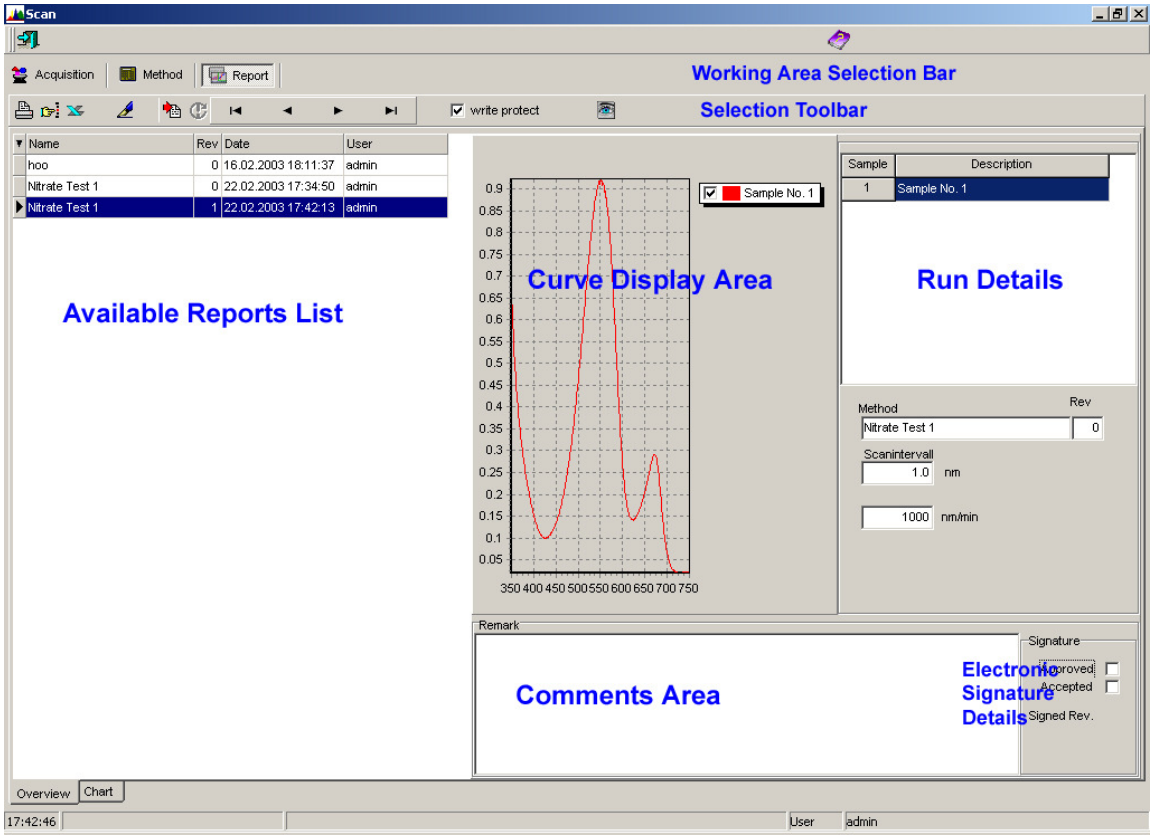
The *Method* page layout is similar for each mode and is shown below. Graphical display functions are again only available in those measuring modes where graphics are actually used, e.g. *Wavelength Scanning*. Other functions such as calibration definition are also not present in every window.



Working Area Selection	Buttons for selection of working window, e.g. *Method*.
Selection Toolbar	Contains buttons for navigating the current method list plus buttons to allow addition or deletion of methods.
Existing Method List	Contains a list of all methods used for the given measuring mode. Scrolling through the list updates automatically the corresponding fields in the parameter definition fields.
Parameter Definition	All parameters necessary for the method are defined and displayed here.
Current Method History	Displays data relevant to the creation and history of each method in the list.

2.3.1.5. The Report Window

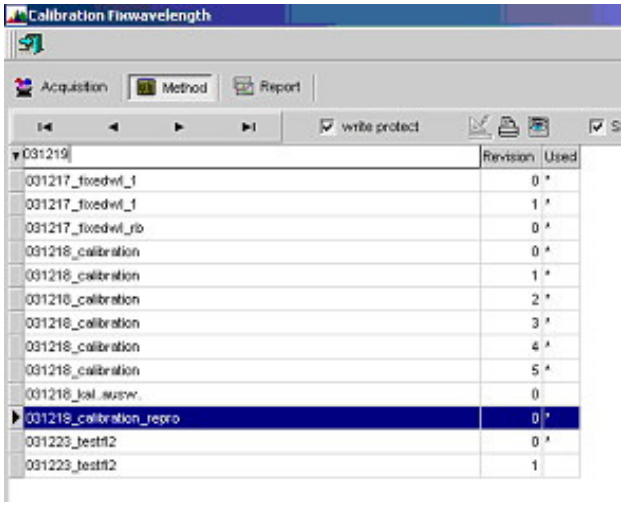
The *Report* page layout is similar for each mode and is shown below. Graphical display functions are again only available in those measuring modes where graphics are actually used.



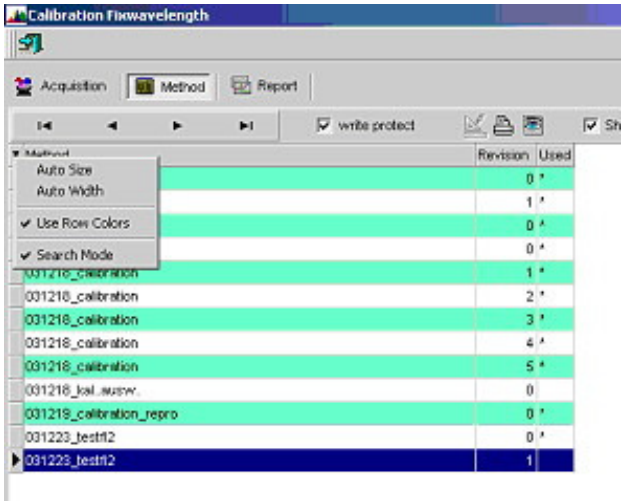
Working Area Selection	Buttons for selection of working window, e.g. *Method*.
Selection Toolbar	Contains buttons for navigating the current list plus buttons to allow archiving or printing of reports.
Available Reports List	Contains a list of all reports available used for the given measuring mode. Scrolling through the list updates automatically the corresponding fields in the results area fields.
Curve Display Area	Shows all curves available for the current report.
Comments Area	Displays data for the samples contained in the current report.
Electronic Signature	Shows details relating to status of electronic signature for a report.

2.3.1.6. Quick Search Function and Row Colouring

In Methods and Reports a quick search function may be used to quickly find the required file. Therefore, click on the fixed row to enter the name of the file. It will be highlighted automatically.



Also, by clicking on the small arrow in the left corner of the fixed row, the rows may be coloured.



2.3.2. Starting a measurement

The **"Start"** button on the main menu bar is used in all methods to start measurement of one to ten samples. All parameters defined in the selected method are then used for a measurement.

Measurement can be stopped at any time by pressing the **"Stop"** button on the main menu bar. All data measured up to that point is valid and can be stored and used for further processing.

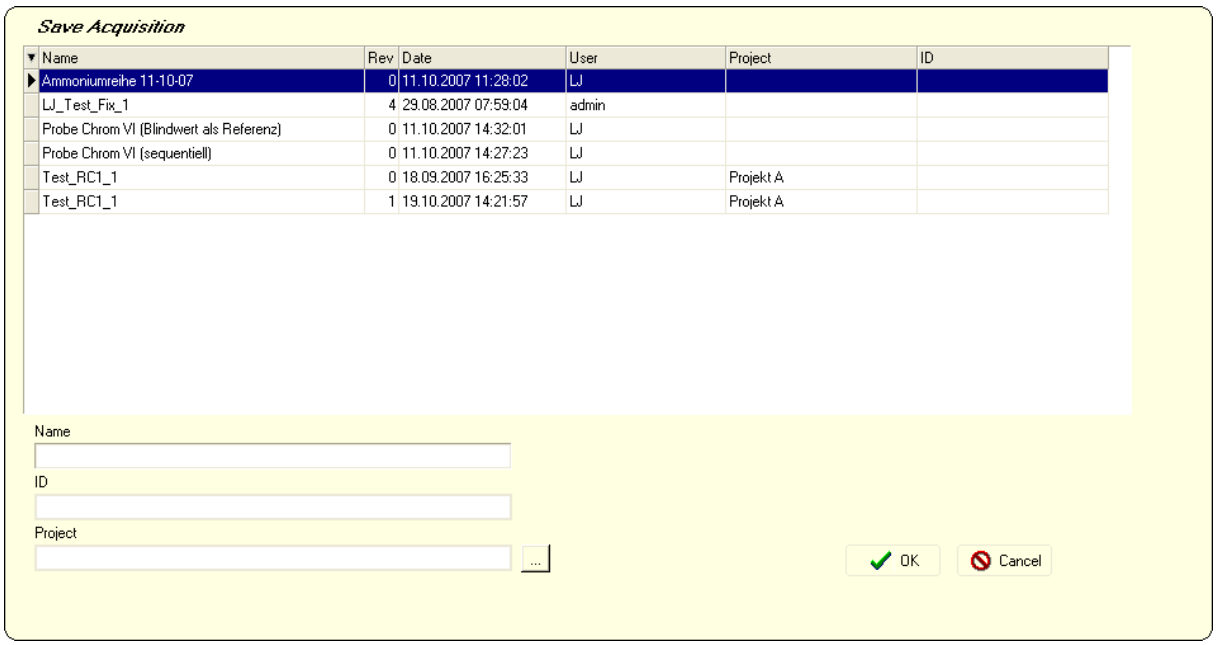
2.3.3. Recalculation

The calculations are made automatically as part of the acquisition process in the UVS software. In cases where parameters are changed a recalculation can be forced as described below.

Clicking on the *Calculator* icon on the tool bar is used throughout the software package to initiate a re-calculation of one to ten samples. Only the parameters in the calculate column and the display column of the acquisition parameter set are used for calculation.

2.3.4. Saving data

Clicking on the "**Save**" button on the toolbar allows the currently displayed data to be saved. The following dialogue box appears:



Enter the required file name in the input window , select a project if available and click on the *OK* button.

2.3.5. Loading existing data files

Data which has already been acquired can be viewed via the main *Report* window in any of the measuring modes.

Select the *Report* window by clicking on the *Report* button. The left hand section of the window contains a list of acquired data files which can be viewed and loaded by clicking on the appropriate line.

2.3.6. Data conversion to EXCEL format

Data files can be converted directly to Excel® (*.XLS) format to be read from Excel spreadsheet programs. Excel must be installed for this function to be used. The data will be transferred directly to Excel and can then only be saved and processed within Excel.

Caution: *This data cannot be re-imported into the UVS software and is not subject to any further controls by the UVS software with respect to security considerations for electronic documentation.*

Click on the icon to transfer data to Excel. Excel is opened automatically and the data entered in a worksheet.

2.3.7. Export to Clipboard

Data files in graph format can be exported to the *Windows Clipboard* to be immediately imported into other running programs via the copy-paste mechanism.

Click on the clipboard icon in the graphics toolbar and the curve is exported automatically to the clipboard for further processing.

2.3.8. ASCII Export

For interfacing with a LIMS system, ASCII export is possible from Acquisition and from Report mode.

If the sample set has been stored as a report then the ASCII file gets the same name as the report itself – with the extension ".txt".

These ASCII files can be directly read by the LIMS systems.

2.3.9. Methods

The system will always use a set of parameters called a "*Method*" to execute the data acquisition and measurement step.

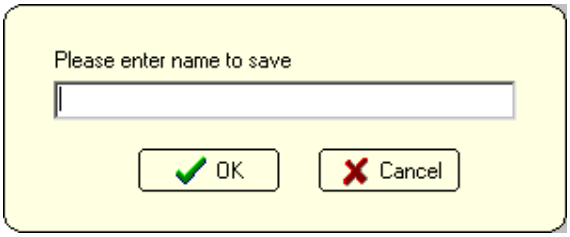
The method file for an acquisition is selected from a drop-down list in the main acquisition window as described below each measuring mode. Simply click on the required method in the list.

Programming and viewing of methods is made from the *Method* screen for each measuring mode. Existing methods are shown in a list in the left-hand window, clicking or scrolling through the list allows an easy overview of the current method in this list.

A new method is programmed by removing the “write-protect” check box tick and clicking on the “ + “ icon. The available functions for each method type are described in the appropriate sections below.

2.3.10. Saving methods

The system prompts for a name for the method to be stored whenever a new method is to be created. Generally methods cannot be simply overwritten because of the tracking system used for CFR Part 11 therefore it is necessary to enter a new name and confirm with *OK*.



Once the parameters for the method have been entered the method is saved by clicking on the green tick in the option tool bar:

2.3.11. Cancel all current activities

Clicking on the *Exit* icon in the top left-hand corner of each screen will return automatically to the start-up screen.

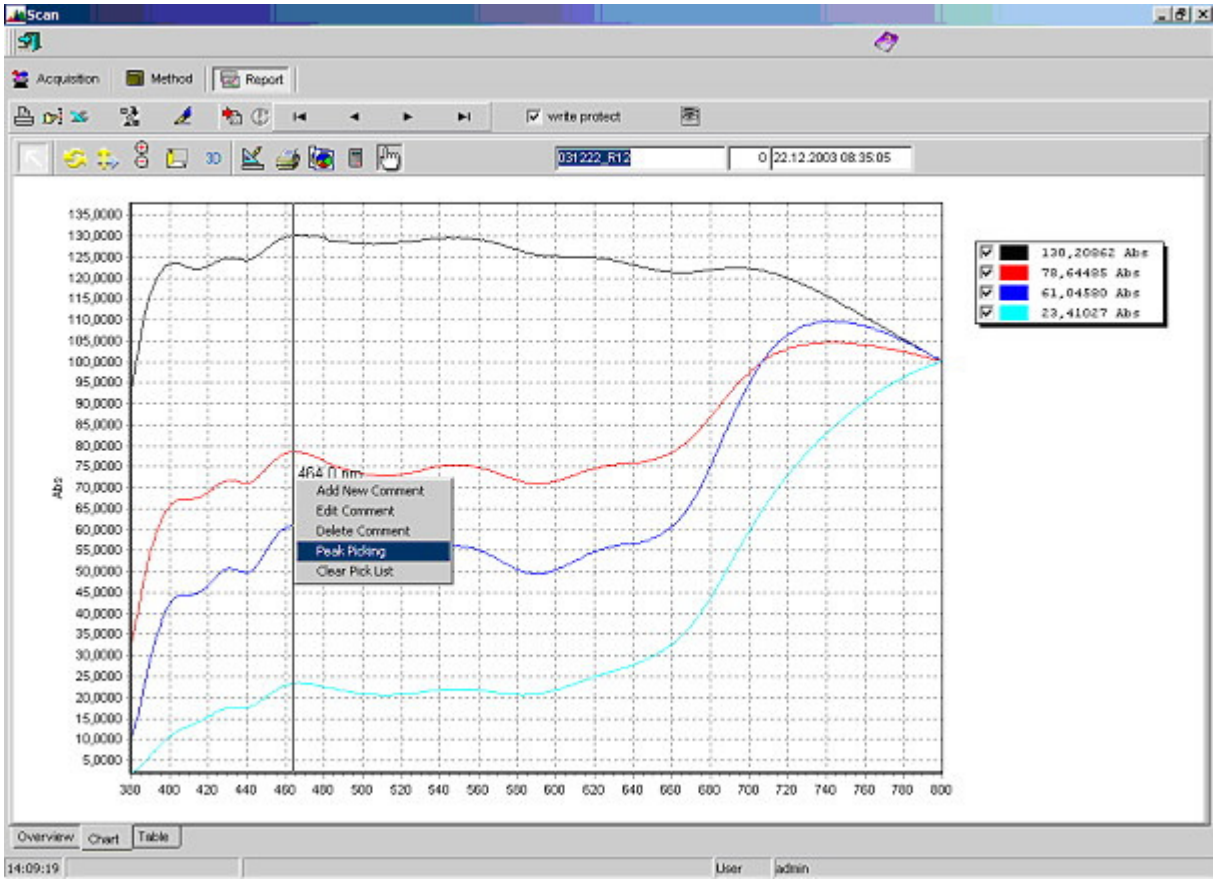
Clicking on the “Stop” button in the acquisition screen will cancel any currently running data acquisition etc.

Caution *If you exit without having saved your data on disk you cannot restore the data. A message will warn you if this situation occurs.*

2.3.12. Activate Cursor and Manual Peak Picking

The *Activate Cursor* icon can be used in *Wavelength Scan*, *Time Drive* and *Auto Rate Assay* methods to quickly overview values of the sample curve on the screen.

In the *Report Overview* window click on the chart tab to obtain the curve display. Click on the *Activate Cursor* icon. A vertical cursor can now be moved across the curve graph and the values for the wavelength are continuously displayed on the cursor line. The arrow used to move the cursor is also used for the position of the Y-axis and values for the current Y-position are continuously updated in the legend window adjacent to the curve.
Additionally, by clicking on the right mouse button, you may add new comments, edit and delete comments.



When the cursor is activated, you may manually pick peaks by clicking the right mouse button and choose *Peak Picking*.
You can also activate or deactivate samples in the legend.

2.3.13. Zooming

Zooming is available for all methods where graphical curve displays, e.g. *Wavelength Scan*, *Time Drive* or *Auto Rate Assay*, are available and is used to magnify a section of the graph.

Simply move the cursor on the graph to the upper left corner of the rectangle to be magnified, press the left button of the mouse and move it to the right while keeping the left button pressed. A rectangle will be shown on the screen indicating the area that will be magnified.

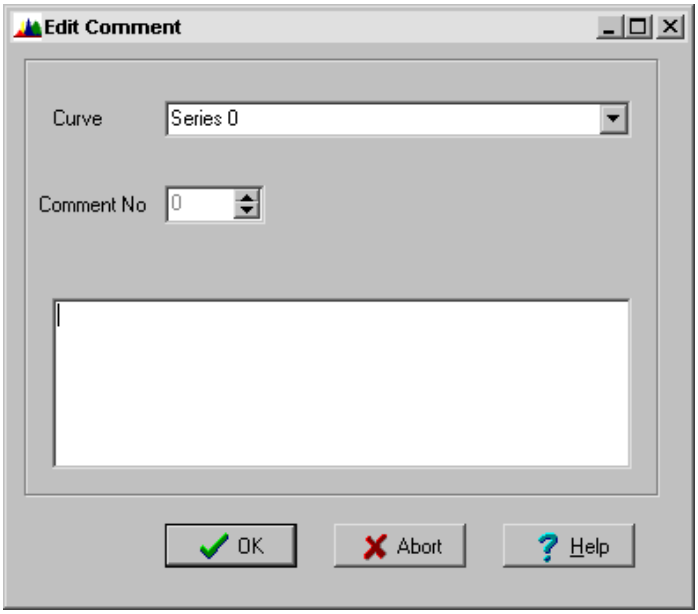
When you reach the lower right corner of your area, release the button and the area selected is zoomed to fill the graph area.

You can repeat the zooming function up to the maximum resolution by repeating the selection of the zoomed area.

To unzoom simply position the cursor on the graph, press the left mouse key, move the cursor to the left and release the left mouse key or double click with left mouse key.

2.3.14. Adding comments to curves

You can add a comment at any point on a curve for documentation purposes. When a curve is displayed on the screen, click the *Activate Cursor* icon in the Graphics toolbar, move the mouse cursor to the point on the curve where the comment should be added and click the right mouse button. A small dialogue box appears offering the choice of adding, editing or deleting a comment. Click on a selection and the appropriate dialogue window will appear:



Input the desired comment text using alphanumeric characters and press "**OK**". The comment will appear directly linked to the curve at the cursor position on the X-axis.

More comments may be added by repeating the same procedure. The comments are numbered and the spin selector by the *Comment No* box can be used when editing or deleting comments in order to select the item to be used.

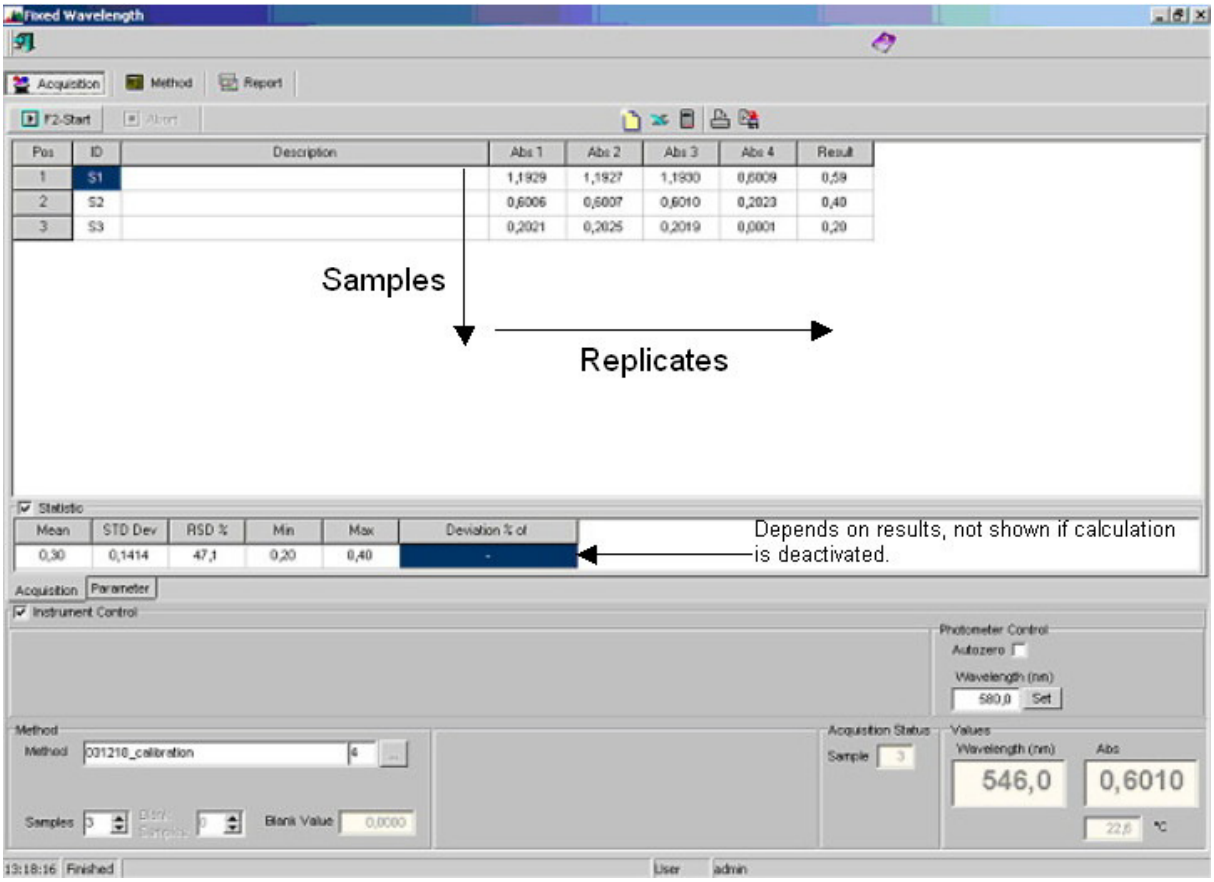
2.4. SYSTEM MODES

This section explains the parameters and gives a step by step measurement example for each system mode. Many parameters are common to all methods but are explained separately for each mode in the interests of clarity.

2.4.1. Fixed Wavelength

2.4.1.1. The Acquisition Screen in Fixed Wavelength

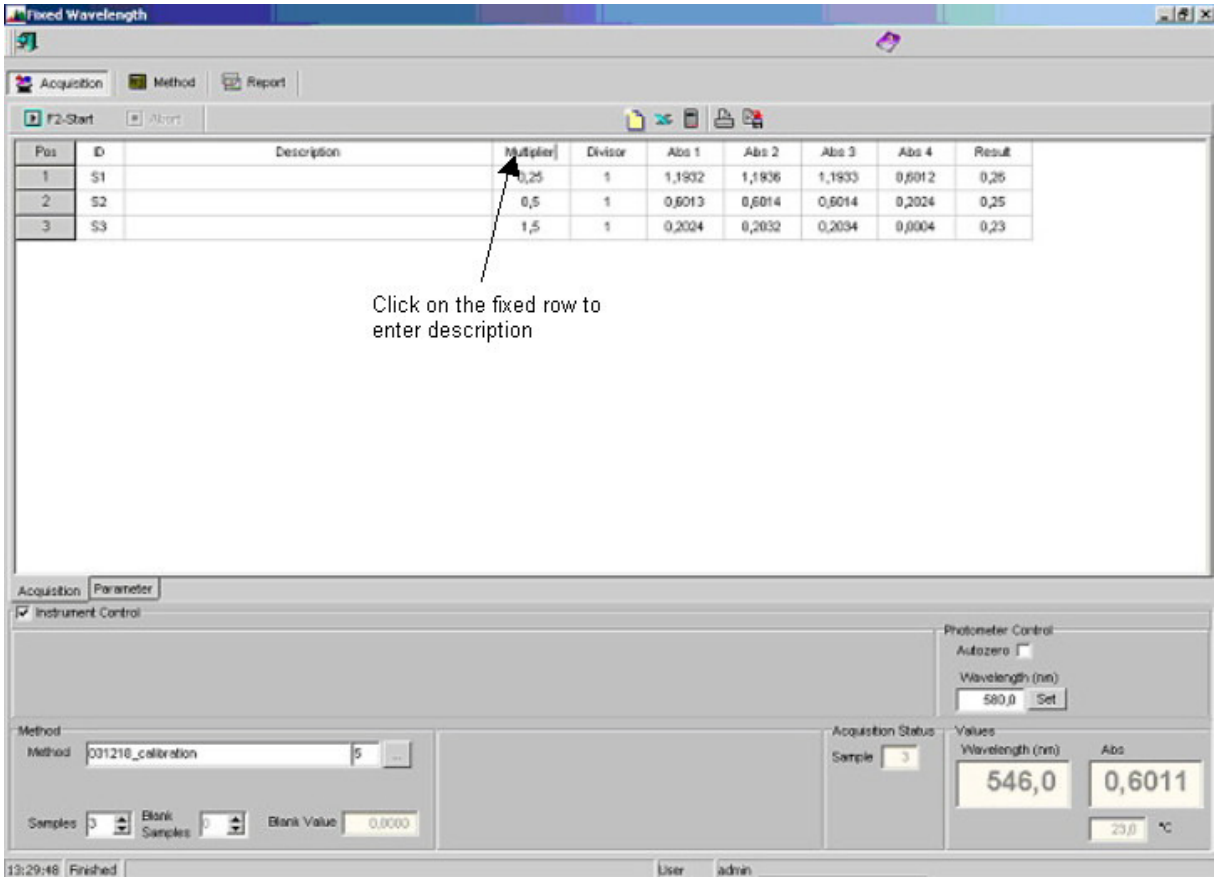
Select **"Fixed Wavelength"** from the main menu to obtain the following display:



This is the acquisition window from which all measurements are started. In this window the following parameters must be selected before starting a measurement:

- Method to be used for the acquisition. The method contains all parameters necessary for the execution of the measurement.
- Numbers of samples to be measured.
- Number of blank samples, measured as the first samples.
- Autozero at start of measurement.
- Load previous saved data from a report

If Individual Multiplier / Divisor is activated in the Method, you may add a multiplication / division factor before the measurement values. Both, multiplier and divisor, have to be defined. The factor not used should therefore be set to “1”. E.g. if you choose the multiplier of 1.7 for a sample, you have to set the respective divisor to 1. The calculation will be applied by clicking on the *Calculate* icon in the selection toolbar. You may also define a description for the factor by clicking on the fixed row to enter description.



2.4.1.1.1. Statistic

If *Calculation* is activated in the *Method*, the calculation of mean, standard deviation, RSD %, min., max. and the deviation percentage of the mean regarding sample no. 1 will be shown.

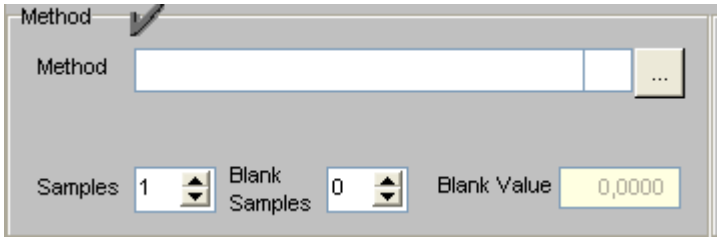
If *Concentration* is activated in the *Method*, a chart is shown with the concentration values and the regression curve.

2.4.1.1.2. Instrument Control

Autozero may be activated before starting a measurement.

2.4.1.1.3. Run parameters

The run parameters are entered in the lower left section of the screen:



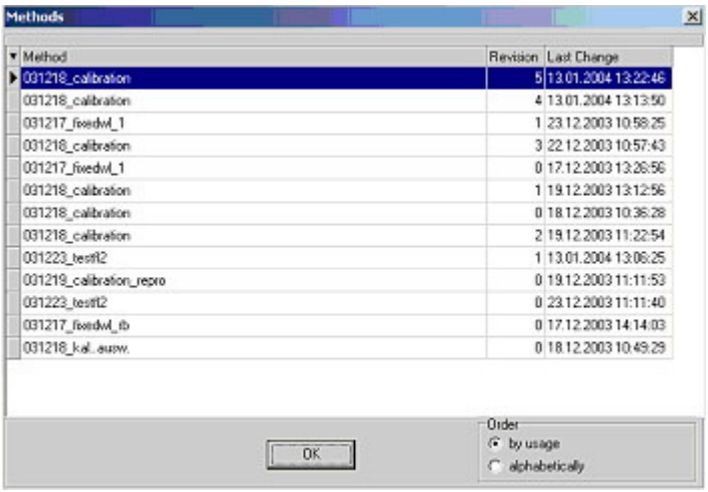
Samples Defines the number of samples to be analysed.

Blank Samples Defines the number of blank samples to be measured, blank samples are always expected at the start of a run. The value of the measured blank is subtracted from the actual measured value of the sample prior to calculation of concentration etc. If more than one blank is defined then the system calculates the average blank value for the blanks and then subtracts this from the actual measured sample values.

Method The method box contains the name of the method and, directly adjacent, the actual revision number of that method. The method is selected from a separate window which opened by clicking on the button adjacent to the revision box.

Checkbutton Press this button to accept the number of samples, the sample grid will also created.

Thermo System Surveys the temperature of the sample

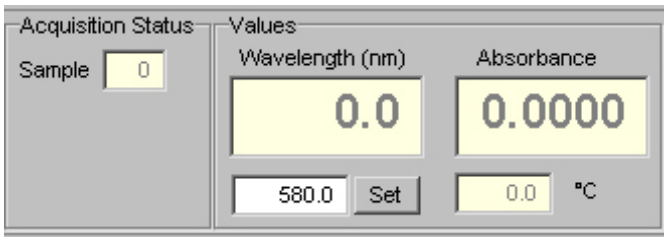


This window contains a list of all available methods including all revisions of the method and the date of last modification. The order of the shown methods may be selected by ticking “by usage” or “alphabetically” in the lower right corner of the screen. Selection is made by highlighting the required line and then clicking on *OK*.

Cell Changer The operating mode of the cell changer and the actual position can be defined here before starting a measurement series.

Note : During the Dialogbox *‘Please insert replicate’* it is possible to move the cell changer with the ‘+’ and ‘-‘ key.

2.4.1.1.4. System Status



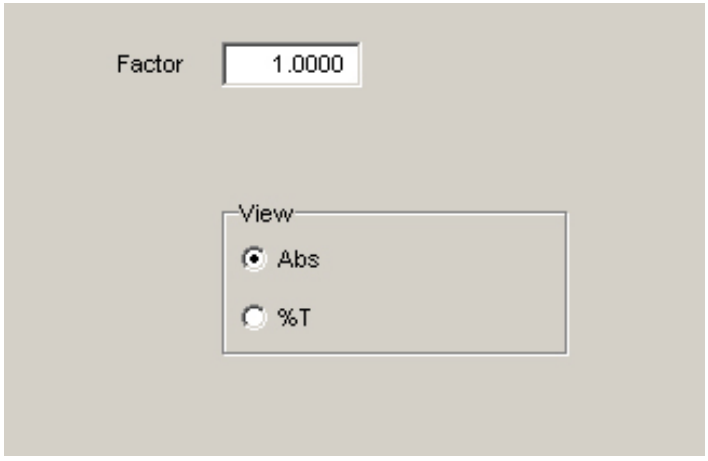
The lower right section of the display contains the actual status of the system and displays the following parameters:

- Current sample being measured.
- Actual wavelength.
- Actual absorbance value.
- Temperature (where applicable).

In addition the lower right panel also allows manual setting of wavelength in order to allow rapid monitoring of the unit.

2.4.1.2. Parameters in Fixed Wavelength Acquisition

Clicking on the parameter tab in the acquisition allows access to the following parameters:

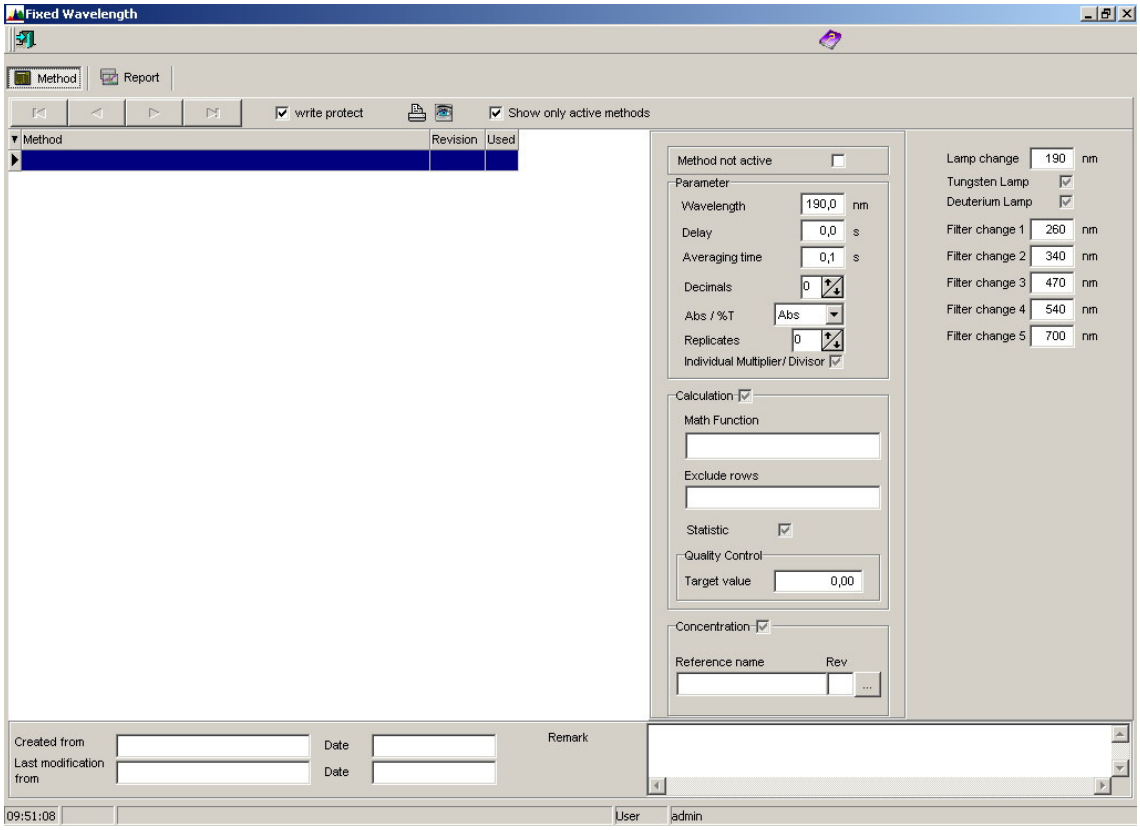


Factor The factor can be used to calculate concentrations or other values if the response of the substance measured is known. In this case use of a calibration file would not be necessary.

View These checkboxes permit toggling between absorbance and transmission values for the display of the acquired data. The data is always saved according to the definitions in the method independent of this setting.

2.4.1.3. The Method in Fixed Wavelength

Click on the *Method* button in the upper left corner to open the *Method* window:



The left-hand window contains a list of all existing methods including revisions and an indication of whether they have been used already or not.

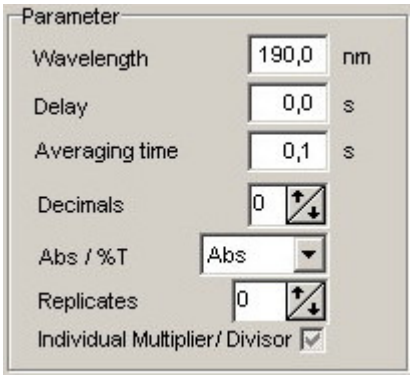
Caution: *If measurements have been used, the method will be locked and can no longer be changed. However, they can be used for later measurements or modified with revision control. Such methods are indicated by a " * " in the " used " column list.*

A new method can be created from within the method section by using the '+' button. In order to do this it is first necessary to uncheck the write-protect checkbox.

The system will first prompt for name under which the new method will be saved. Once this has been defined all other parameters can be entered.

2.4.1.3.1. Acquisition parameters

Method not active Inactivate, and thus hide the current *Method* by checking this box.



Wavelength Defines the wavelength to be used for the measurement.

Delay time The instrument will wait for the selected delay time after the MEASURE key is pressed to start the actual measurement.

Averaging time Defines the time the instrument uses to collect data for calculation of a mean value for one reading. A long averaging time is useful to reduce noise when measuring at high absorbance values.

Decimals Defines the amount of decimals for the measurement values.

Abs / %T Selection permits definition of the mode to be used. The user can select between either absorbance or transmission.

Replicates Defines the number of acquisitions per sample to determine the resulting mean.
E.g.: Replicates = 0 : only one acquisition per sample
Replicates = 1 : two acquisitions per sample

Individual Multiplier/Divisor By checking this box, a separate dilution factor (multiplier) and weight factor (divisor) can be defined for each sample.

2.4.1.3.2. Common Parameters

The right-hand panel contains common parameters, which are required for every system and user method. They will be stored and recalled along with all other parameters.

Lamp change This parameter defines the lamp change wavelength. The deuterium lamp is used for all wavelengths below the lamp change wavelength. The tungsten halogen lamp is used for all wavelengths above the lamp change wavelength.

Tungsten lamp When checked the tungsten lamp will be switched on and used according to the setting for the lamp change.

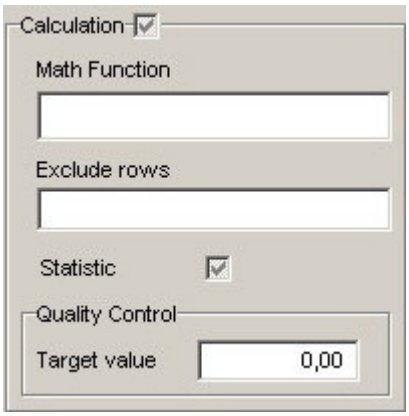
Deuterium lamp When checked the deuterium lamp will be switched on and used according to the setting for the lamp change.

Filter change (1-5) This parameter defines the wavelength used to switch the filter.

Bandwidth Selects the spectral bandwidth of the spectrophotometer.

Cell changer Defines the operating mode of the cell changer (if fitted).

2.4.1.3.3. Calculation



Calculation Deactivate *Calculation* for normal acquisitions without any special calculation. Activate *Calculation* for special calculations defined under *Math Function*.

Math Function This function depends on the grid of absorbance values. Enter the calculation desired.
Examples: ((A1-A2)-(A4-A3))*F ; ((A1-A2)-(A1,1-A2,1))*F

Table Matrix Example I:

Abs 1	Abs 2	Abs 3	Abs 4	Result
A1	A2	A3	A4	V

Table Matrix Example II:

Abs 1	Abs 2	Abs 3	Result
A1,1	A2,1	A3,1	W
A1,2	A2,2	A3,2	X
A1,3	A2,3	A3,3	Y
A1,4	A2,4	A3,4	Z

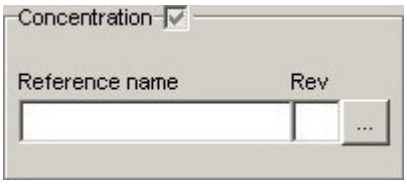
The first number indicates the different measurements of one sample, the second number indicates the sample number. E.g.: A2,1 is the first replicate of the first sample, A1,2 is the first measured value of sample no. 2.
F = factor given with the acquisition window
Other operators (*,/,+,sqr,...) may be entered.

Exclude rows Enter the rows to be excluded. The calculation of results (mean, std dev,...) will not use these rows for calculation.

Target value This is a value for the statistics window. The deviation will be calculated with the mean value and the target value.

Note: *Calculation and Concentration checkboxes cannot both be ticked at the same time. An error message will be shown during saving of the method.*

2.4.1.3.4. Concentration



If the *Concentration* checkbox is ticked, the system will use the defined calibration reference for the calculation of the concentration values based on the results of the measurement.
By clicking the "..."-button next to the *Rev* Box, you can select the calibration file to be used. The boxes show the *Reference name* of the selected file and its revision number (*Rev*).

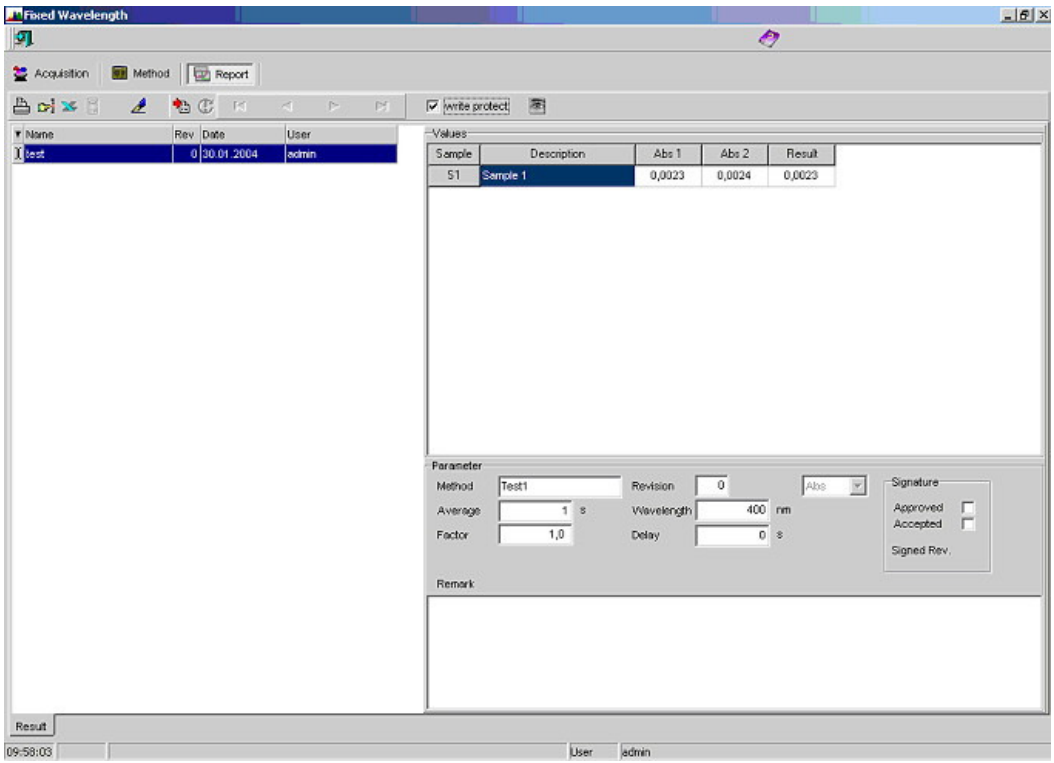
Note: Calculation and Concentration checkboxes cannot both be ticked at the same time. An error message will be shown during saving of the method.

2.4.1.3.5. Audit Trail in Fixed Wavelength Method

Click on the Audit Trail icon to view the audit trail window for the method.

2.4.1.4. The Report Screen in Fixed Wavelength

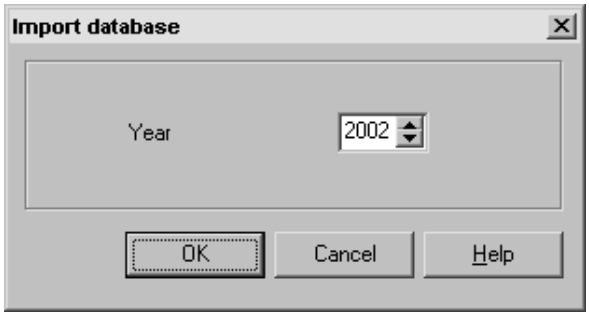
Click on the *Report* button in the upper left corner to open the *Report* window:



The left-hand window contains a list of all available reports, the right-hand window contains the results in the upper section and the main parameters for the measurement in the lower part. Each report can be viewed by scrolling through the left-hand list.

2.4.1.4.1. Printing

Click on the *Print* icon to obtain a print preview of the selected report, which will always contain all measurements. The report can be printed by clicking on the *Print* icon on the preview page.



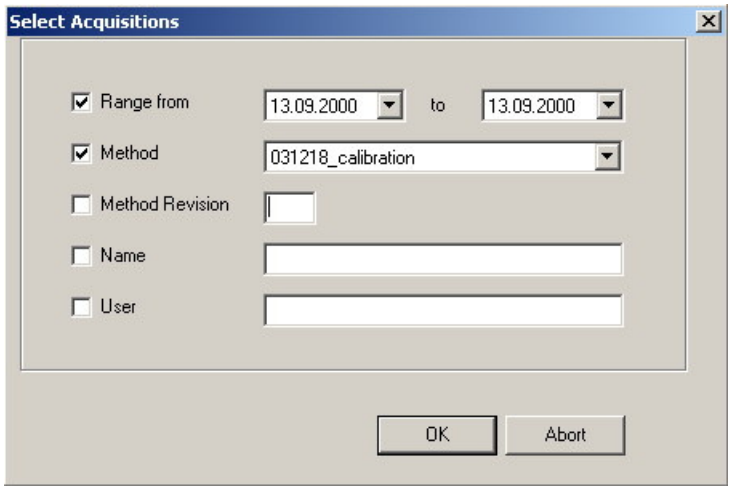
2.4.1.4.2. Importing a report from the database

Click on the *Import* icon to access earlier reports in the extracted database. A dialogue window for selection of the database will be opened:

2.4.1.4.3. Filtering the report list

The report list in the left window will become very long with time and it may be necessary to filter the list so that only those files of interest to a user are actually shown. This is carried out using the *Select Report* icon.

Click on the *Select Report* icon and a dialogue window appears, which allows selection of a view by date, method, user or name:



The appropriate checkbox must be checked and, where applicable, either a date or name selected. Clicking on *OK* will cause only those reports which satisfy all selected criteria to be shown in the list of available reports.

2.4.1.4.4. Audit Trail in Fixed Wavelength Report

Click on the *Audit Trail* icon to view the audit trail window for the report.

2.4.1.5. Calculations in Fixed Wavelength

Fixed Wavelength contains four basic calculation methods for final result determination:

- Linear regression
- Quadratic regression
- Blank
- Factor

In *Fixed Wavelength* the *Blank* and *Factor* calculations are executed automatically without the need to create a calibration file:

Blank The measured values for sample blank is subtracted from the measured value of each sample measured.

Factor The actual value obtained from the measurement is always multiplied by the factor parameter. This is accessible by clicking on the *Parameter* tab in the acquisition screen.

The actual calculation is based on the following formula:

$$R = F * (VM_{sample} - VM_{blank})$$

Where R = Result, F = Factor and VM represents the measured values obtained for sample and blank respectively.

Recalculation after, for example, changing the factor value is possible at any time by clicking on the *Calculator* icon.

2.4.1.6. Concentration in Fixed Wavelength

In simple cases the *Result* obtained above can be used as a concentration value if the *Factor* has been defined and zero concentration corresponds to zero absorbance.

Using the calibration function, it is possible to calculate concentration values based on a previously determined calibration curve. This method offers the advantage that any absorbance offset is compensated for and that the final result is given in the desired units in the report print-outs.

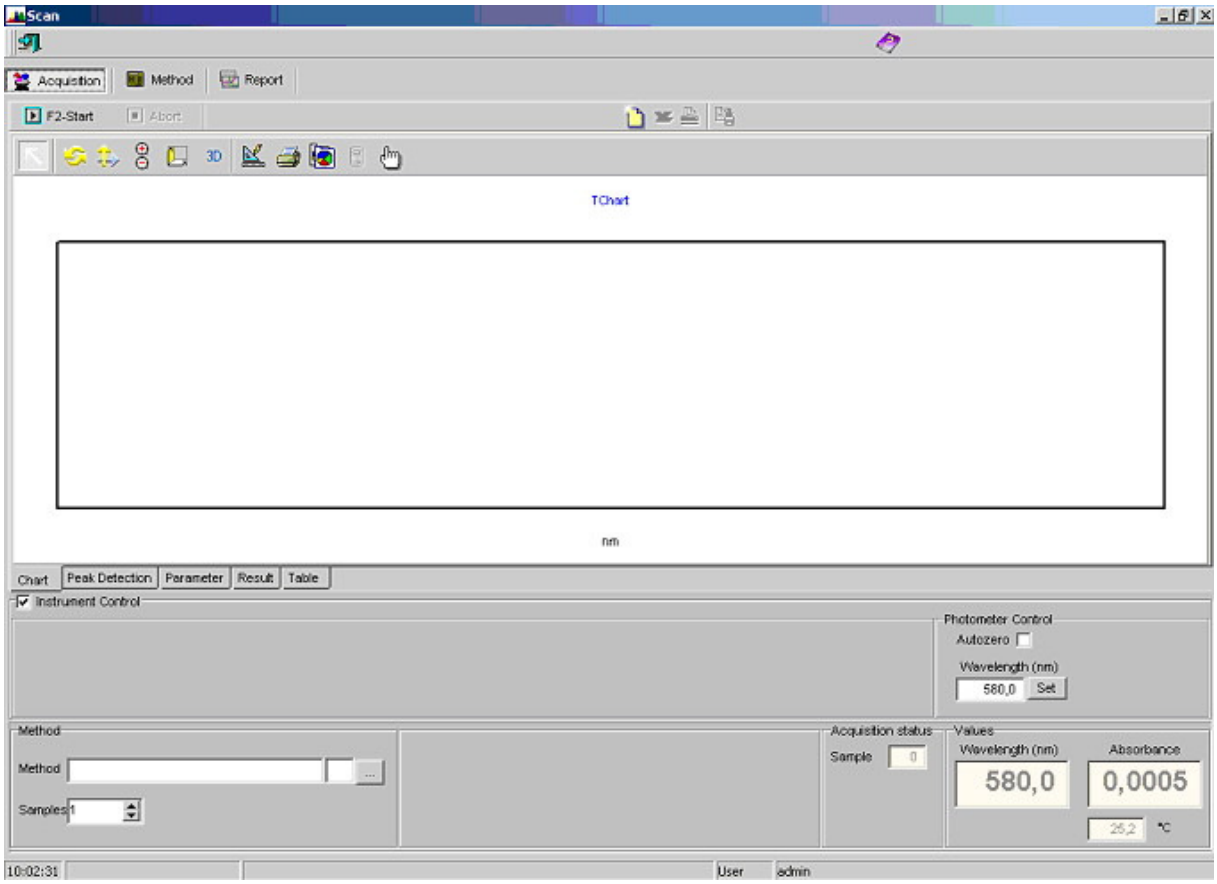
The calibration uses the value obtained for the *Result* (see above) and converts this value to a corresponding concentration value in units, which are defined as part of the calibration file.

A more detailed description of the *Calibration* function is given in a separate section within this document.

2.4.2. Wavelength Scan

2.4.2.1. The Acquisition Screen in Wavelength Scan

Select **"Wavelength Scan"** from the main menu to obtain the following display:

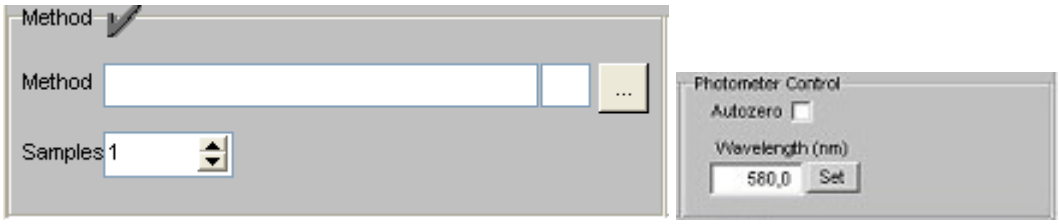


This is the acquisition window from which all measurements are started. In this window the following parameters must be selected before starting a measurement:

- Method to be used for the acquisition. The method contains all parameters necessary for the execution of the measurement.
- Numbers of samples to be measured.
- *Autozero* at start of measurement.
- Load previous saved data from a report

2.4.2.1.1. Run parameters

The run parameters are entered in the “Method” panel and in the “Photometer control” panel:

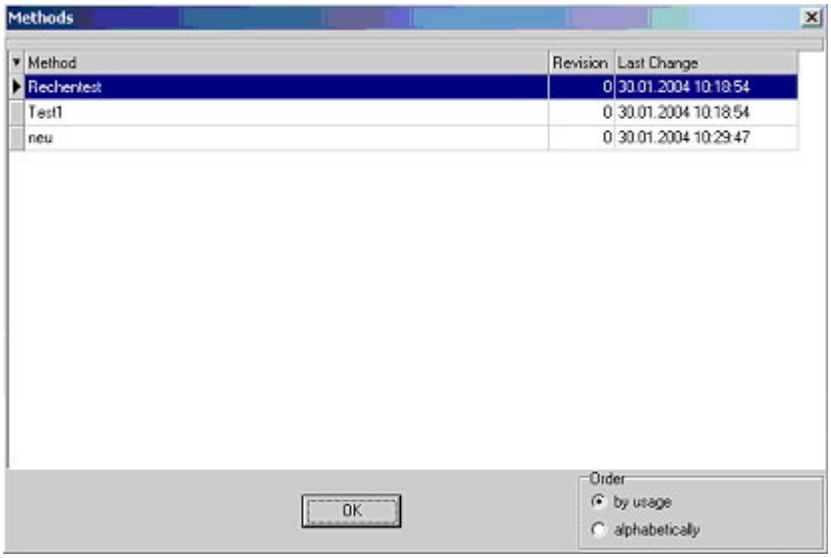


Samples Defines the number of samples to be analysed.

Checkbutton Press this button to accept the number of samples, the sample grid will also created.

Autozero Defines whether an autozero should be executed prior to the start of a measurement.

Method The method box contains the name of the method and, directly adjacent, the actual revision number of that method. The method is selected from a separate window which opened by clicking on the button adjacent to the revision box:



This window contains a list of all available methods including all revisions of the method and the date of last modification. Selection is made by highlighting the required line and then clicking on *OK*.
The order of Methods may be displayed by usage or alphabetically.

Wavelength A certain wavelength may be chosen manually and set immediately in order to allow rapid monitoring of the unit.

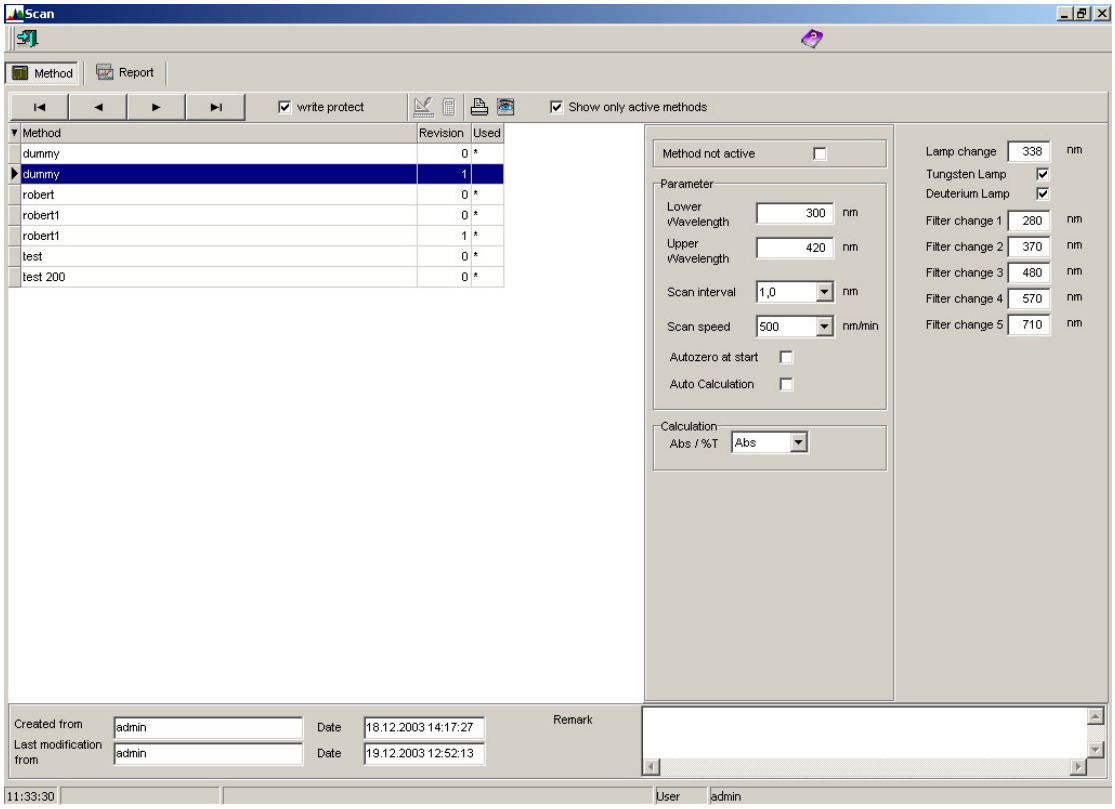
2.4.2.1.2. System Status

The lower right section of the display contains the actual status of the system and displays the following parameters:

- Current sample being measured.
- Actual wavelength.
- Actual absorbance value.
- Temperature (where applicable).

2.4.2.2. The Method in Wavelength Scan

Click on the *Method* button in the upper left corner to open the *Method* window:



The left-hand window contains a list of all existing methods including revisions and an indication of whether they have been used already or not.

Caution: *If measurements have been used, the method will be locked and can no longer be changed. However, they can be used for later measurements or modified with revision control. Such methods are indicated by a " * " in the " used " column list.*

A new method can be created from within the method section by using the '+' button. In order to do this it is first necessary to uncheck the write-protect checkbox.

The system will first prompt for name under which the new method will be saved. Once this has been defined all other parameters can then be entered.

2.4.2.2.1. Acquisition parameters

Method not active Inactivate, and thus hide the current *Method* by checking this box.

Lower Wavelength Defines the lower wavelength for the wavelength range to be used for the measurement.

Upper Wavelength Defines the upper wavelength for the wavelength range to be used for the measurement.

Scan Interval This parameter (also called sampling interval in other instruments) defines the wavelength step between two measured data points.

Scan Speed Defines the wavelength drive speed to be used for the measurement. Scanning speeds can be selected between 5 and 5000 nm/min. If you choose dynamic scan speed, the instrument will automatically optimise the scan speed to suit the slope of your sample.

Autozero If checked, an autozero will be made for each sample beforestarting the scan.

Auto Calculation If checked, the calculation for peak detection, smoothing etc. starts automatically after acquisition using the defined parameters.

2.4.2.2.2. Common Parameters

The right-hand panel contains common parameters, which are required for every system and user method. They will be stored and recalled along with all other parameters.

Lamp change This parameter defines the lamp change wavelength. The deuterium lamp is used for all wavelengths below the lamp change wavelength. The tungsten halogen lamp is used for all wavelengths above the lamp change wavelength.

Tungsten lamp When checked, the tungsten lamp will be switched on and used according to the setting for the lamp change.

Deuterium lamp When checked, the deuterium lamp will be switched on and used according to the setting for the lamp change.

Filter change (1-5) This parameter defines the wavelength used to switch the filter.

Bandwidth Selects the spectral bandwidth of the spectrophotometer.

Cell changer Defines the operating mode of the cell changer (if fitted).

2.4.2.2.3. Calculation

The calculation selection permits definition of the mode of calculation to be used. The user can select between either absorbance or transmission.

2.4.2.2.4. Curve Parameters in the Wavelength Scan Method

Opens an edit dialogue for defining curve parameters and related formatting.

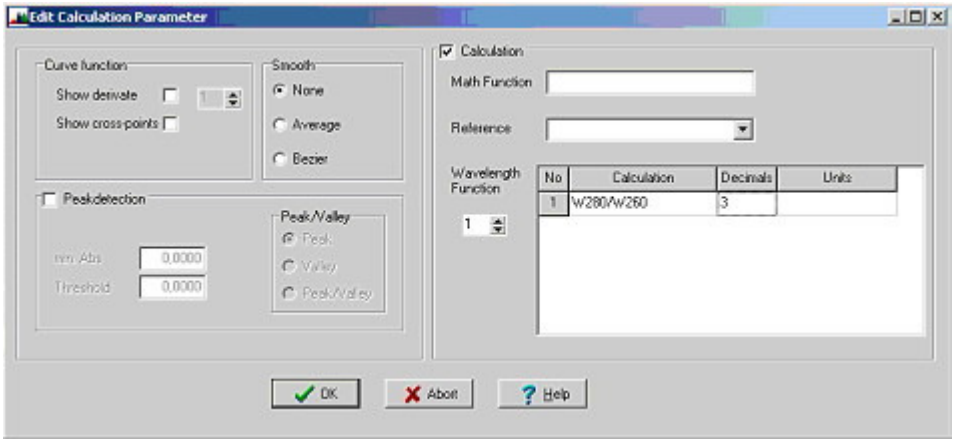
In *Wavelength Scan* the curve parameters can be linked to a method and then define the appearance and properties of the curve such as colours, overlay format, scaling etc.

Functions defined here will be included and stored with the method and thus used for any acquisition executed utilising that method.

Formatting options using this function are described in a separate section of this document.

2.4.2.2.5. Calculation Parameters in the Wavelength Scan Method

Click on this icon to open the calculation dialogue window for the method:



By activating the *Calculation* box, a mathematical function or/and a wavelength function may be implemented.

The *Math Function* may be defined with or without a reference file.
E.g.: S-R Subtract reference from all samples
S+R Add reference to all samples
S*1.2 Multiply all samples with 1.2 (Format 1.2 or 1,2 depends on windows)

If individual references should be subtracted in WL Scan mode (e.g. to subtract the reference from the same cuvette) then the Calculation can be defined in the following way:

- Tick the “Calculation”
- Define the Math. Function “S-R”
- Under “No. of references” define the number of reference runs that should be subtracted from the current runs.

Example:

When an automatic cell changer is in use, then 8 individual blank runs should be subtracted from 8 sample scans afterwards.

- Select 8 references
- Measure the 8 reference runs first
- Add the samples into these 8 cuvettes
- Start again using 8 samples

Then the first 8 references are being automatically subtracted from the following 8 samples.

To use the *Wavelength Function*, choose the number of functions and then enter the wavelength and a mathematical function to have a calculated result.
E.g.: W280/W260
W250*1.2
W300-W350
Nested functions are possible, too.

Some of the calculation functions shown in the dialogue above are described in more detail in the section on Calculation within this document. Functions defined above will be included and stored with the method and thus used for any acquisition executed utilising that method.

The wavelength range can be limited for the calculation of the maxima and minima.

Examples:

WL scan was executed in the wl range from 220 to 500 nm.

MIN[250;300] provides the lowest signal value within the WL range 250 to 300 nm, even if the scan was executed from 220 to 500 nm.

MAX[250;300] provides the highest signal value within the WL range 250 to 300 nm, even if the scan was executed from 220 to 500 nm.

MIN provides the lowest signal value over the entire scan range from 220 to 500 nm.

MAX provides the highest signal value over the entire scan range from 220 to 500 nm.

In addition the new functions **MINL** and **MAXL** indicate the related wavelength in a similar way:

Examples:

WL scan was executed in the wl range from 220 to 500 nm.

MINL[250;300] provides the wavelength for the lowest signal value within the WL range 250 to 300 nm, even if the scan was executed from 220 to 500 nm.

MAXL[250;300] provides the wavelength for the highest signal value within the WL range 250 to 300 nm, even if the scan was executed from 220 to 500 nm.

MINL provides the wavelength for the lowest signal value over the entire scan range from 220 to 500 nm.

MAXL provides the wavelength for the highest signal value over the entire scan range from 220 to 500 nm.

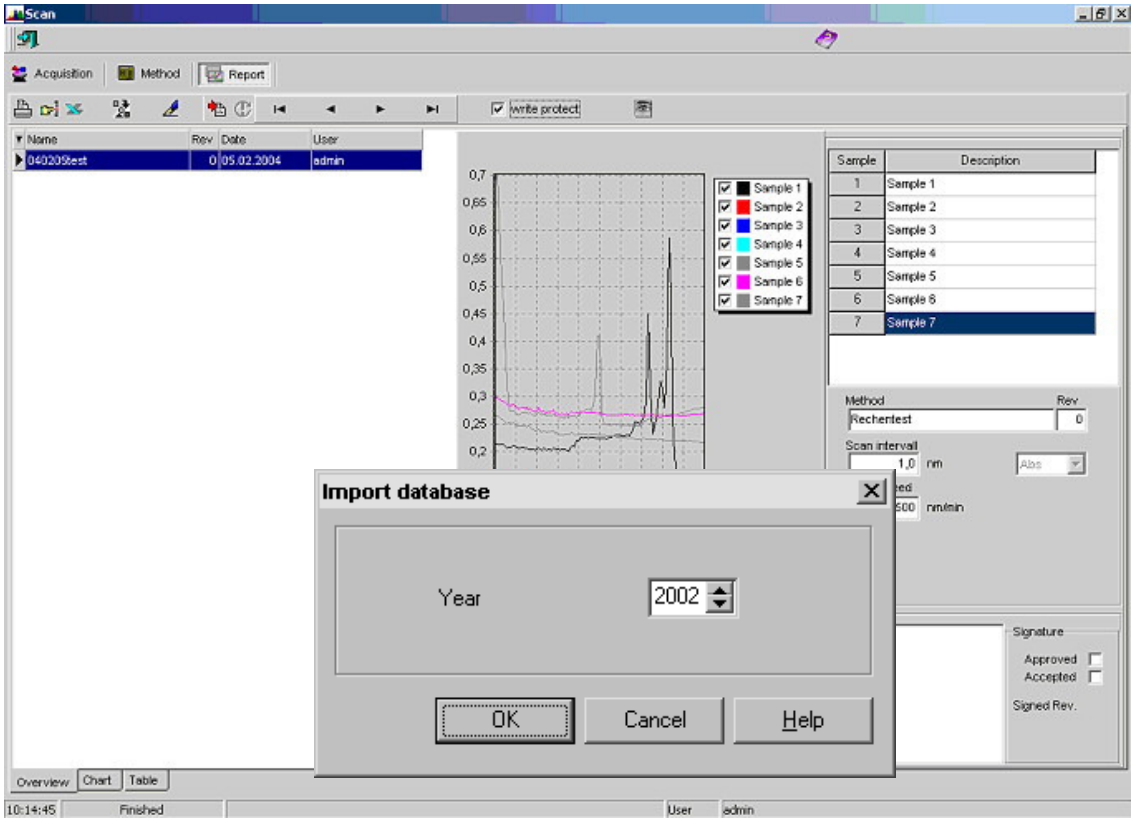
2.4.2.2.6. *Audit Trail in Wavelength Scan Method*

Click on the *Audit Trail* icon to view the audit trail window for the method.

2.4.2.3. The Report Screens in Wavelength Scan

2.4.2.3.1. The "Overview" Report Screen

Click on the *Report* button in the upper left corner to open the *Report* window:



The display obtained is the “Overview” screen, clicking on the “Chart” tab will display the chart as the main item which can be manipulated or edited as required.

The left-hand window contains a list of all available reports, the right-hand window contains the results in the upper section and the main parameters for the measurement in the lower part. Each report can be viewed by scrolling through the left-hand list.

2.4.2.3.2. Printing

Click on the *Print* icon to obtain a print preview of the selected report, which will always contain all measurements. The report can be printed by clicking on the *Print* icon on the preview page.

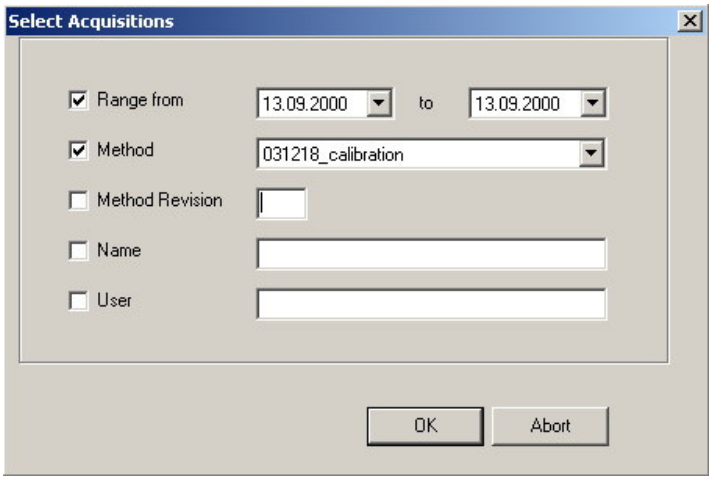
2.4.2.3.3. Importing a report from the database

Click on the *Import* icon to access earlier reports in the archived database. A dialogue window for selection of the database will be opened:

2.4.2.3.4. Filtering the report list

The report list in the left window will become very long with time and it may be necessary to filter the list so that only those files of interest to a user are actually shown. This is carried out using the *Select Report* icon.

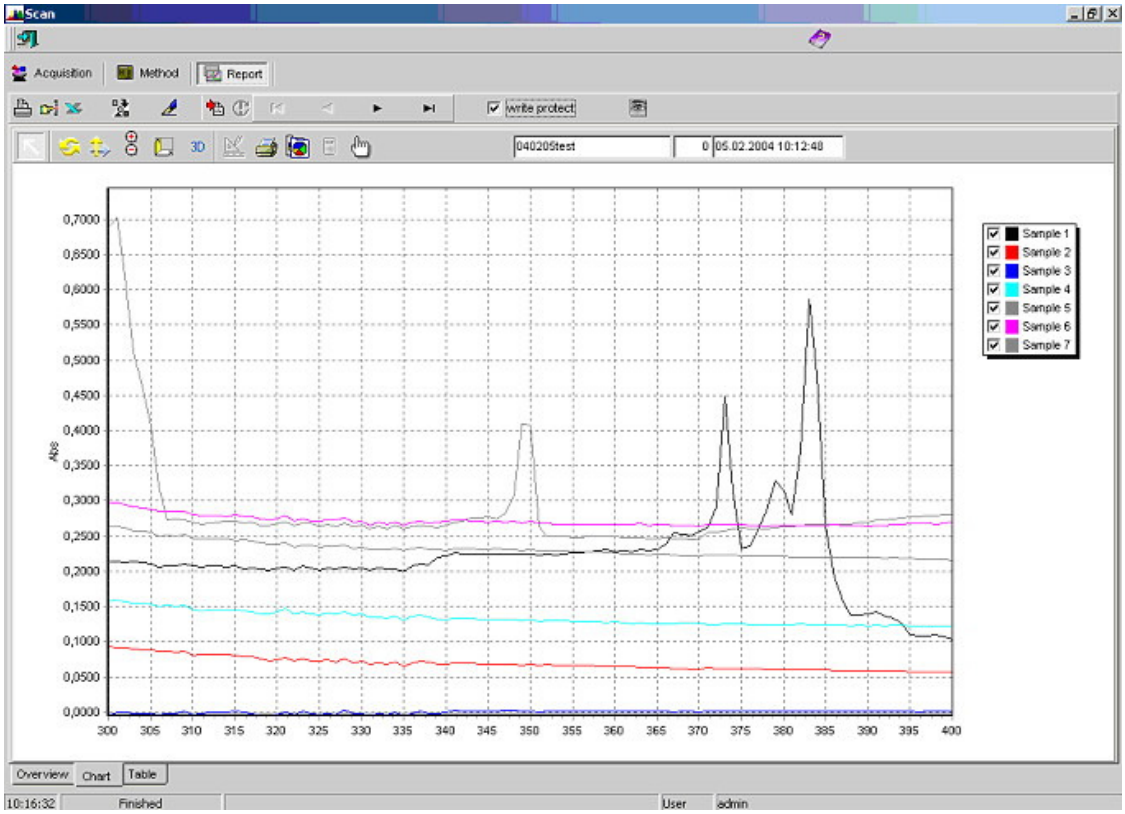
Click on the *Select Report* icon and a dialogue window appears, which allows selection of a view by date, method, user or name:



The appropriate checkboxes must be checked and, where applicable, either a date or name entered. Clicking on *OK* will cause only those reports which satisfy all selected criteria to be shown in the list of available reports.

2.4.2.3.5. The "Chart" Report Screen

Clicking on the "Chart" tab will open a new screen containing the curve in a form which can be edited:



Curves may be displayed as overlays, individual curves can be removed from the overlay if required by clicking the checkboxes shown as part of the legend on the right of the curve.

Navigation arrows are available to move between the various reports contained in the list without the need to return to the *Overview* screen.

The name of the currently displayed curve set including the revision is shown in the box display immediately above the curve display.

In *Chart* mode a range of new functions is available to the user for manipulating the presentation and properties of the current curve.

2.4.2.3.6. "Chart" Report Screen Functions

A graphics toolbar is available within the *Chart report screen*:

The use of the icons in the graphics toolbar allow direct manual manipulation of the currently displayed chart. The function of the individual icons is described briefly below:

Shows position of values on X- and Y-axis and allows to manually pick peaks and to add, edit or delete comments.

Opens the calculation dialogue window.

Exports a curve to the *Windows clipboard* for further processing.

Prints the curve as a single sheet report. Formatting of the report is described in a separate section of this document dealing with curve format.

Opens the edit dialogue for formatting functions. See the separate section of this document dealing with curve format for more details.

Converts chart format to a 3D display. The icon functions as a toggle switch between a 2D and 3D display.

Click on this icon to control the depth of the 3D display using the mouse cursor. Clicking on this icon automatically converts the display format to 3D, return to the 2D display via the 3D icon button.

Double function icon allowing zooming of the complete curve.

Click on this icon to move the complete curve display using the mouse cursor. Clicking on this icon automatically converts the display format to 3D, return to the 2D display via the 3D icon button.

Click on this icon to rotate the complete curve display using the mouse cursor. Clicking on this icon automatically converts the display format to 3D, return to the 2D display via the 3D icon button.

Clicking on this icon will return the function of the mouse cursor to normal thus allowing use of the normal zooming functions etc. in 3D displays.

2.4.2.3.7. Audit Trail in Wavelength Scan Report

Click on the *Audit Trail* icon to view the audit trail window for the report.

2.4.2.4. Calculations in Wavelength Scan

The curve calculation modes are generally embedded in the method and are described above and in detail in the *Calculation* section.

Recalculation after, for example, changing a *Peak Detection* parameter is possible at any time by clicking on the *Calculator* icon followed by election of the parameter within the dialogue window.

2.4.2.5. Peak Detection

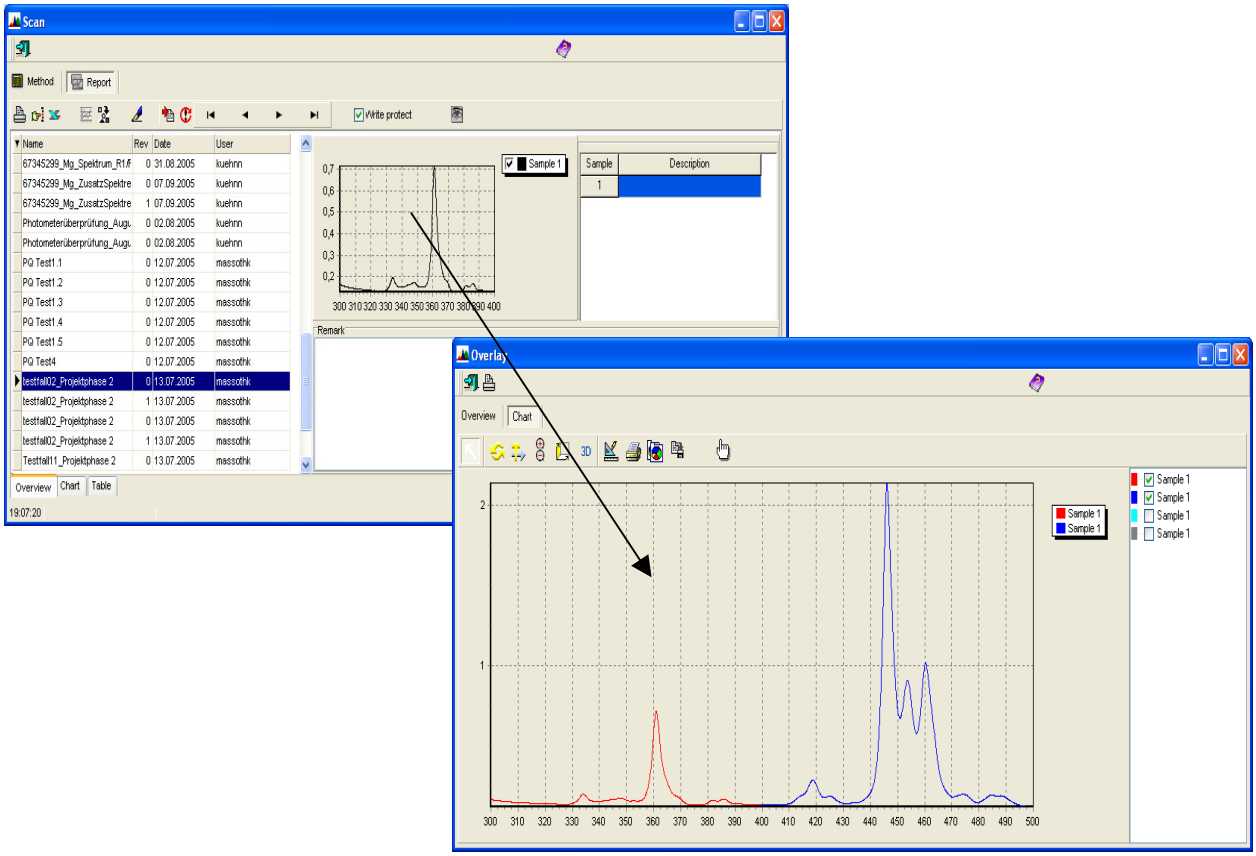
Clicking on the peak detection tab will show the list of wavelength and absorbance values for the detected peaks.

2.4.2.6. Overlay

Overlay is a feature to collect several charts together, even the methods are not the same.

Clicking the overlay button a window called overlay opens. Move to the overview chart, press the left mouse button, move to the overlay window and release the mouse button (drag and drop) .

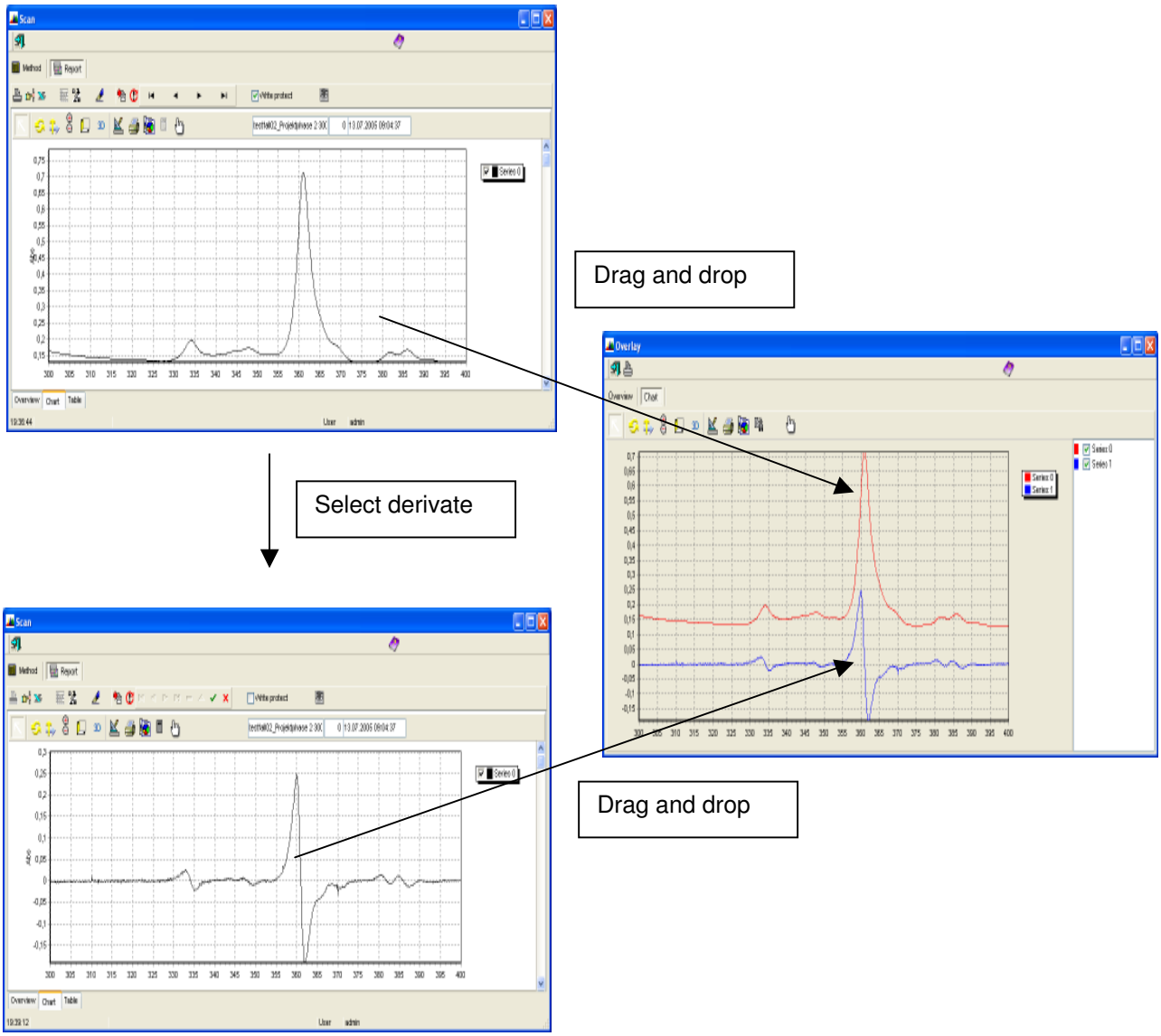
Pressing the save button the overlay will be saved.



Another way to overlay is to start from the chart:

Press **shift and left** mouse button while dragging to the overlay window. Now you can modify the chart and put the result into the overlay.

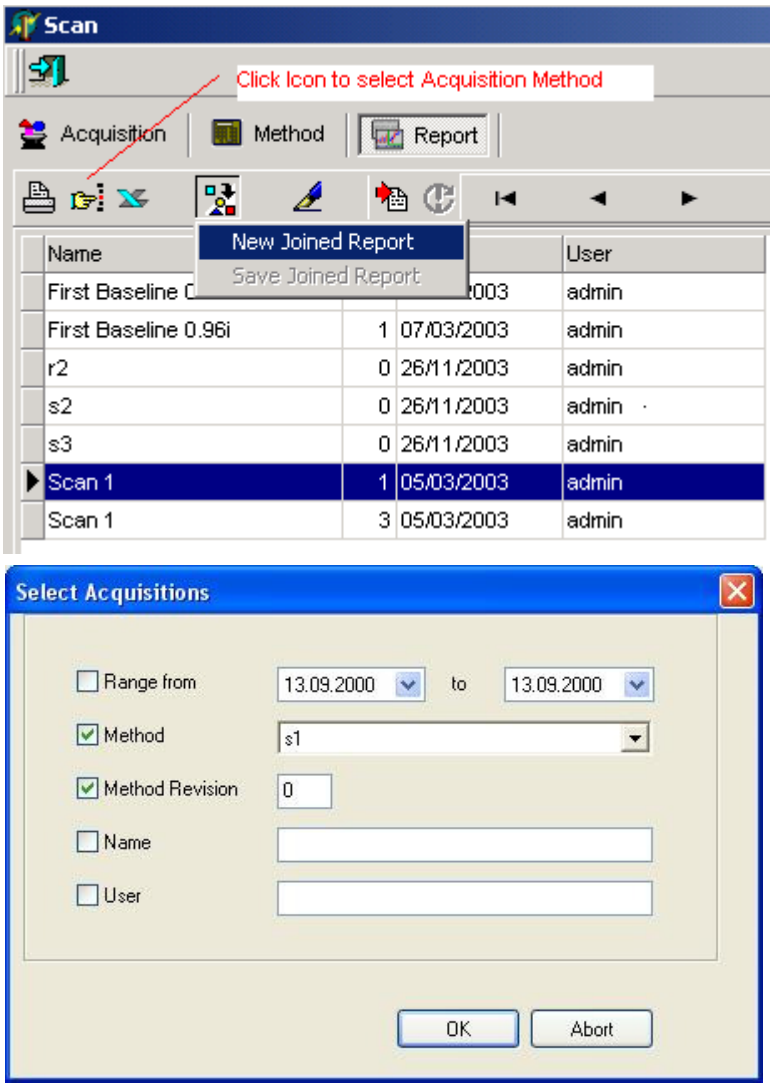
E.g original curve and derivate.



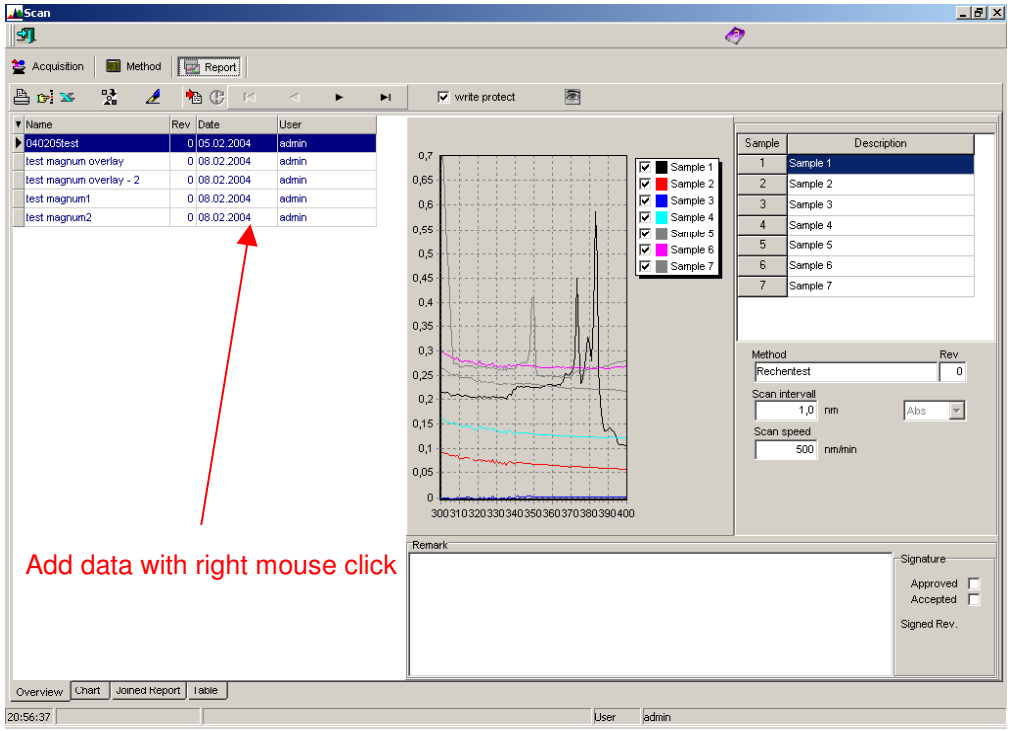
2.4.2.7. Joined Reports

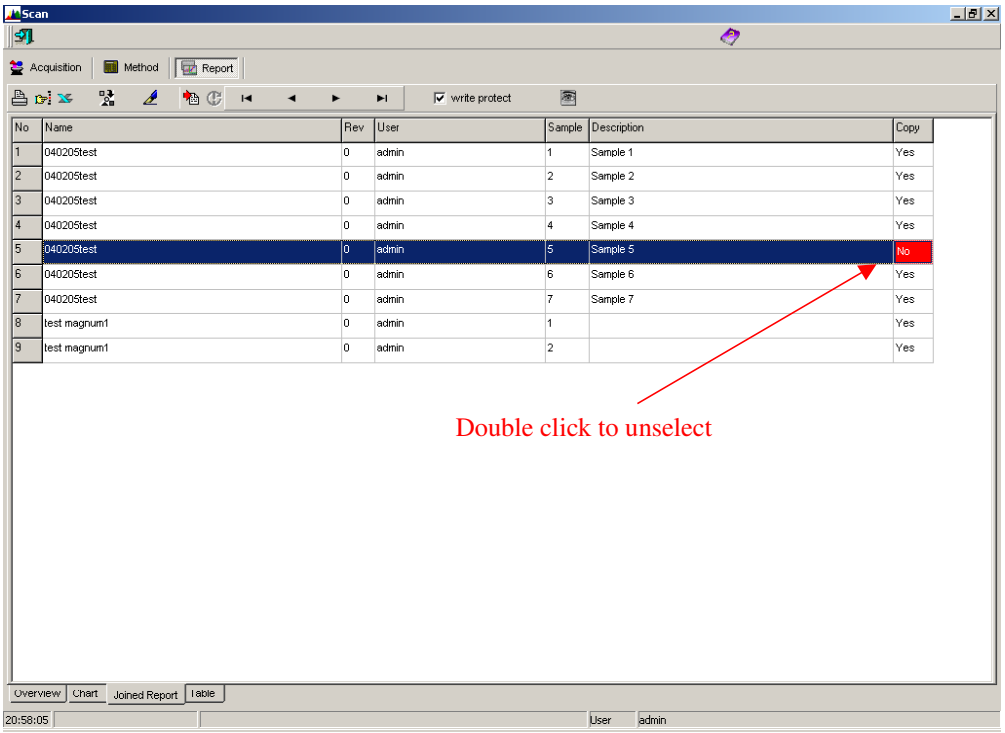
The “Joined Report” option offers the possibility the overlay of spectra from different runs of the same method after the reports have been saved.

To use the Join Report Option click on “New Joined Report” icon and then choose the method that you want to join your reports from. Please not that only data acquired with identical method and revision of method can be overlayed and make sure that select and enter both values.



Select dataset from the Overview List and then add the file by using the right mouse button. The selection of datasets can be monitored in the card “Joined Report” during the process. After the completed selection of your datasets save the created Joined Report File.
The overlay is saved as a normal report, so that all mathematical and graphical functions are available.

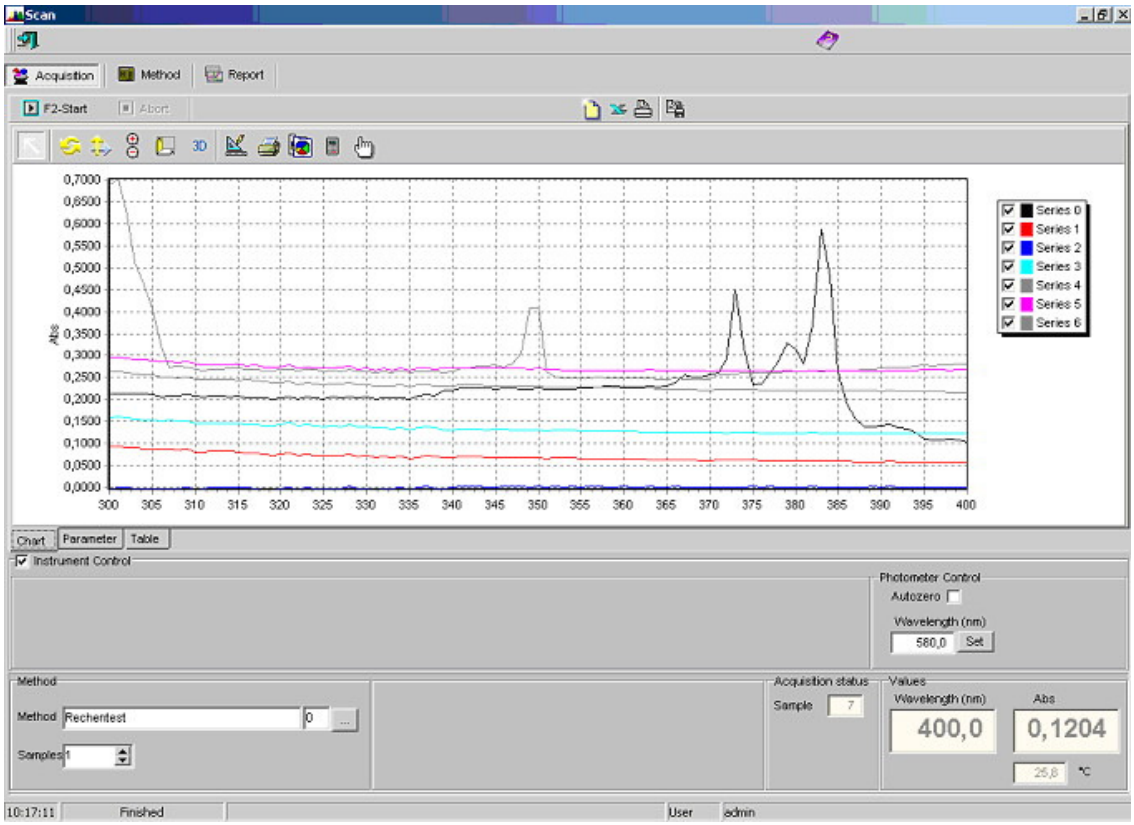

Scan
Acquisition
Method
Report
write protect
Name
Rev
Date
User
040205test 0 05.02.2004 admin
test magnum overlay 0 08.02.2004 admin
test magnum overlay - 2 0 08.02.2004 admin
test magnum1 0 08.02.2004 admin
test magnum2 0 08.02.2004 admin
Sample 1
Sample 2
Sample 3
Sample 4
Sample 5
Sample 6
Sample 7
Description
Method
Rechentest
Scan intervall
1,0 nm
Scan speed
500 nm/min
Remark
Signature
Approved
Accepted
Signed Rev.
Overview
Chart
Joined Report
Table
20:56:37
User
admin
Add data with right mouse click


Scan
Acquisition
Method
Report
write protect
No Name Rev User Sample Description Copy
1 040205test 0 admin 1 Sample 1 Yes
2 040205test 0 admin 2 Sample 2 Yes
3 040205test 0 admin 3 Sample 3 Yes
4 040205test 0 admin 4 Sample 4 Yes
5 040205test 0 admin 5 Sample 5 No
6 040205test 0 admin 6 Sample 6 Yes
7 040205test 0 admin 7 Sample 7 Yes
8 test magnum1 0 admin 1 Yes
9 test magnum1 0 admin 2 Yes
Overview
Chart
Joined Report
Table
20:58:05
User
admin
Double click to unselect

2.4.2.8. Wavelength Scan Measurement Example

Scanning measurement of one blank and five samples using the cell changer.

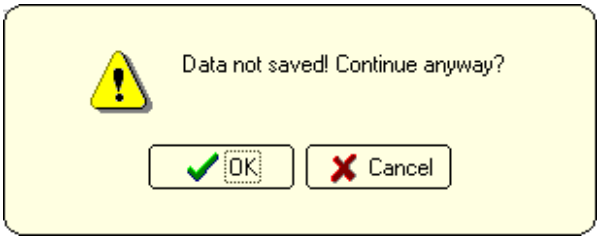
Select the method to be used and set the number of samples to 6. Insert the samples into the cell changer and start the measurement by pressing the *Start* button. The measured curves are displayed in real time during acquisition. A 3D display (see below) may be used to give better clarity if the curves are very similar for each sample. The final window will look similarly like this:



Note: *If you are not using a cell changer, you will be prompted for the next sample after each sample has been measured. The final appearance of the screen remains unchanged.*

Individual curves may be removed from the overlay display by clicking the checkboxes in the legend on the right of the curve.

If you repeat the measurement you will always measure the selected number of samples (6 in our example) until you change the *Samples* parameter. The system will prompt if the previously run sample data has not been saved beforestarting a new run:



Click on *OK* to start the next acquisition run or on *Cancel* to return to the original data set.

Printing

Click on the *Print* icon to obtain a preview of the printed report, which will always contain all measurements. If the result is acceptable the report can be printed by clicking on the *Print* icon on the preview page.

The function “Add peak detection to document” includes as well the peak detection list before the graphics printout, even for “small document” selection.

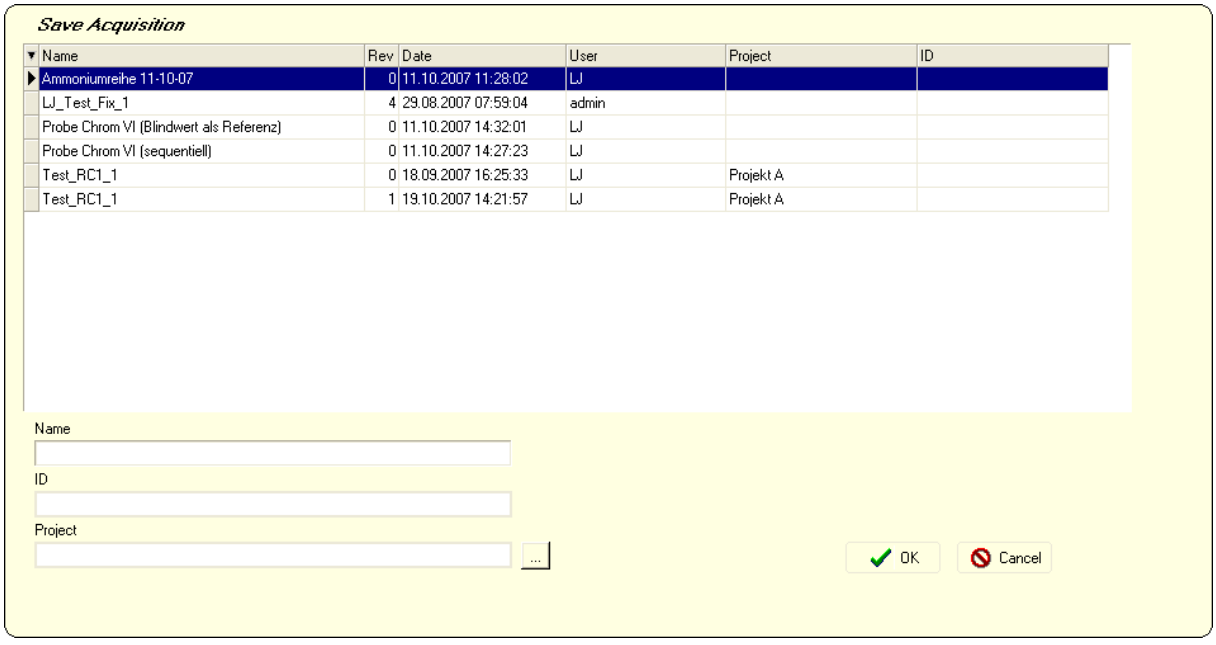
When the function “Add peak detection to document” has been selected and a calculation formula is defined then the calculation is printed on top and the peak detection list follows as second object before the graphic element.

Print Document with Single Curve

If several scans were included in one graphic curve then it was sometimes difficult to identify the curves and all related elements.
The new print option “Print Document with Single Curve” allows to automatically printing each curve separately (one sheet per curve) or per curve pair, if individual reference curves were selected. The peak detection list and the calculations list contains as well only the values for the current single curve, the next page contains then the next curve with the related peak detection and calculation results etc.

Saving

Click on the *Save* icon and the system will prompt for a file name:

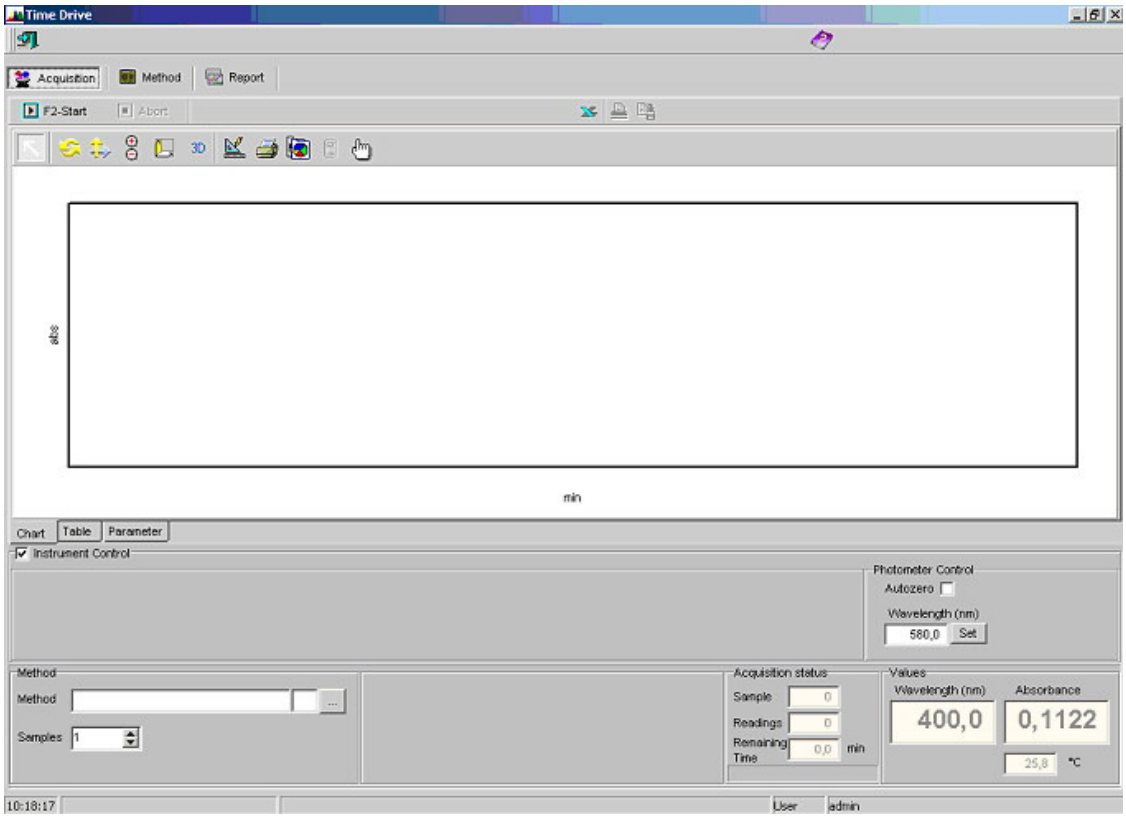


Select the project, if availabe, enter the file name and click on *OK*.

2.4.3. Time Drive

2.4.3.1. The Acquisition Screen in Time Drive

Select **"Time Drive"** from the main menu to obtain the following display:

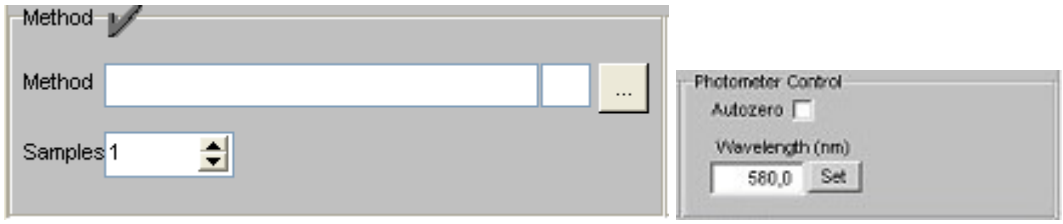


This is the acquisition window from which all measurements are started. In this window the following parameters must be selected before starting a measurement:

- Method to be used for the acquisition. The method contains all parameters necessary for the execution of the measurement.
- Numbers of samples to be measured.
- *Autozero* at start of measurement.
- Load previous saved data from a report

2.4.3.1.1. Run parameters

The run parameters are entered in the "Method" panel and in the "Photometer control" panel:

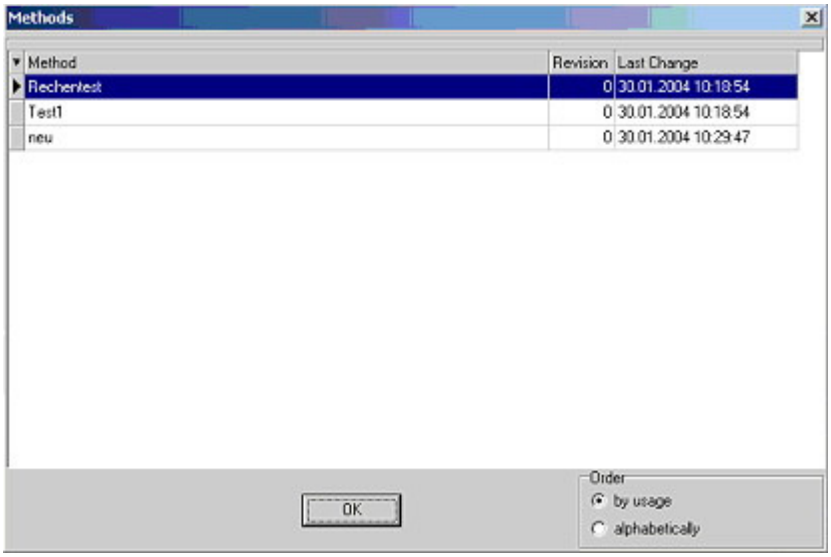


Samples Defines the number of samples to be analysed.

Checkbutton Press this button to accept the number of samples, the sample grid will also created.

Autozero Defines whether an autozero should be executed before starting a measurement.

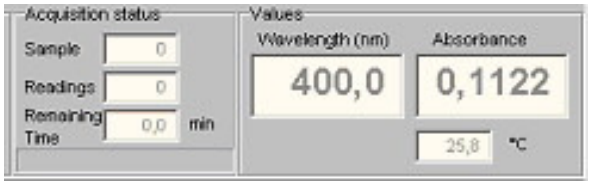
Method The method box contains the name of the method and, directly adjacent, the actual revision number of that method. The method is selected from a separate window which is opened by clicking on the button adjacent to the revision box:



This window contains a list of all available methods including all revisions of the method and the date of last modification. Selection is made by highlighting the required line and then clicking on OK.
The order of Methods may be displayed by usage or alphabetically.

Wavelength A certain wavelength may be chosen manually and set immediately in order to allow rapid monitoring of the unit.

2.4.3.1.2. System Status

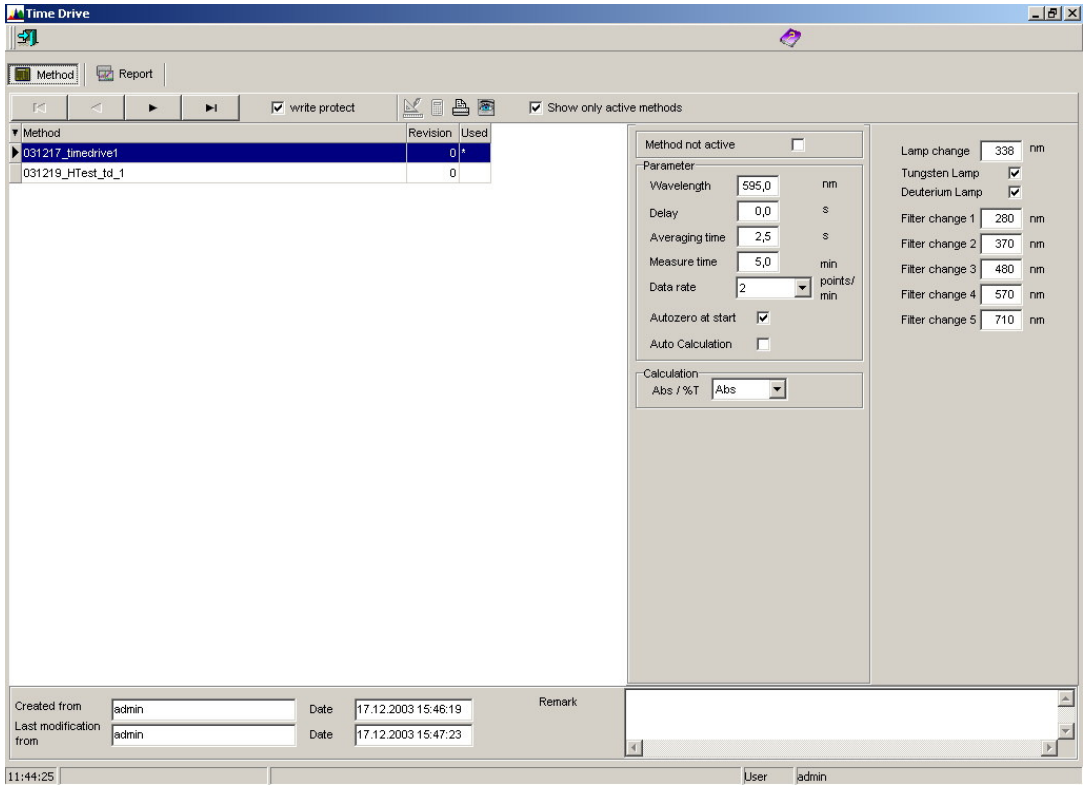


The lower right section of the display contains the actual status of the system and displays the following parameters:

- Current sample being measured.
- No. of Readings
- Remaining Time (also as progress bar)
- Actual wavelength.
- Actual absorbance value.
- Temperature (where applicable).

2.4.3.2. The Method in Time Drive

Click on the *Method* button in the upper left corner to open the *Method* window:



The left-hand window contains a list of all existing methods including revisions and an indication of whether they have been used already or not.

Caution: *If measurements have been used, the method will be locked and can no longer be changed. However, they can be used for later measurements or modified with revision control. Such methods are indicated by a " * " in the " used " column list.*

A new method can be created from within the method section by using the '+' button. In order to do this it is necessary to uncheck the write-protect checkbox.

The system will first prompt for name under which the new method will be saved. Once this has been defined all other parameters can be entered.

2.4.3.2.1. Acquisition parameters

Method not active Inactivate, and thus hide the current *Method* by checking this box.

Wavelength Defines the wavelength to be used for the measurement.

Delay time The instrument will wait for the selected delay time after the MEASURE key is pressed to start the actual measurement.

Averaging time Defines the time the instrument uses to collect data for calculation of a mean value for one reading. A long averaging time is useful to reduce noise when measuring at high absorbance values.

Measure time Defines the actual duration of the measurement in minutes.

Sampling rate Defines the number of data points per minute for the measurement.

Autozero at start Defines whether an autozero is to be executed beforeeach sample run.

Auto Calculation If checked, the calculation for peak detection, smoothing etc. starts automatically after acquisition using the defined parameters.

Calculation mode Calculation and curve portrayal can be in either *Absorbance* or *Transmission* units.

2.4.3.2.2. Common Parameters

The right-hand panel contains common parameters, which are required for every system and user method. They will be stored and recalled along with all other parameters.

Lamp change This parameter defines the lamp change wavelength. The deuterium lamp is used for all wavelengths below the lamp change wavelength. The tungsten halogen lamp is used for all wavelengths above the lamp change wavelength.

Tungsten lamp When checked, the tungsten lamp will be switched on and used according to the setting for the lamp change.

Deuterium lamp When checked, the deuterium lamp will be switched on and used according to the setting for the lamp change.

Filter change (1-5) This parameter defines the wavelength used to switch the filter.

Bandwidth Selects the spectral bandwidth of the spectrophotometer.

Cell changer Defines the operating mode of the cell changer (if fitted).

2.4.3.2.3. Calculation

The calculation selection permits definition of the mode of calculation to be used. The user can select between either absorbance or transmission.

2.4.3.2.4. Curve Parameters in the Time Drive Method

Opens an edit dialogue for defining curve parameters and related formatting.

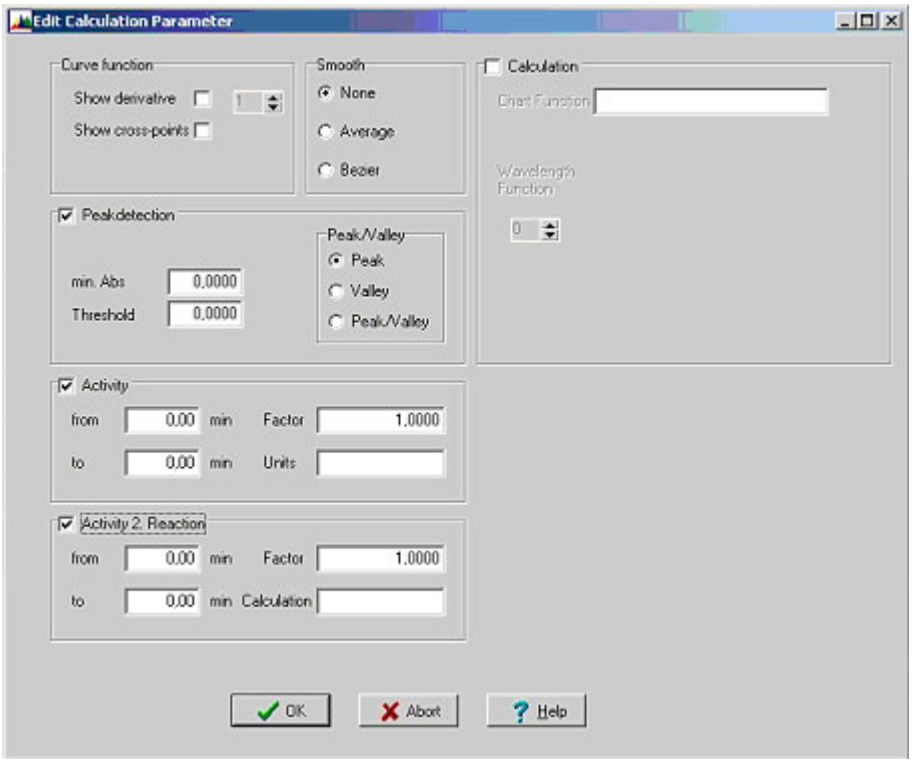
In *Time Drive* the curve parameters can be linked to a method and then define the appearance and properties of the curve such as colours, overlay format, scaling etc.

Functions defined here will be included and stored with the method and thus used for any acquisition executed utilising that method.

Formatting options using this function are described in a separate section in this document.

2.4.3.2.5. Calculation Parameters in the Time Drive Method

Click on this icon to open the calculation dialogue window for the method:

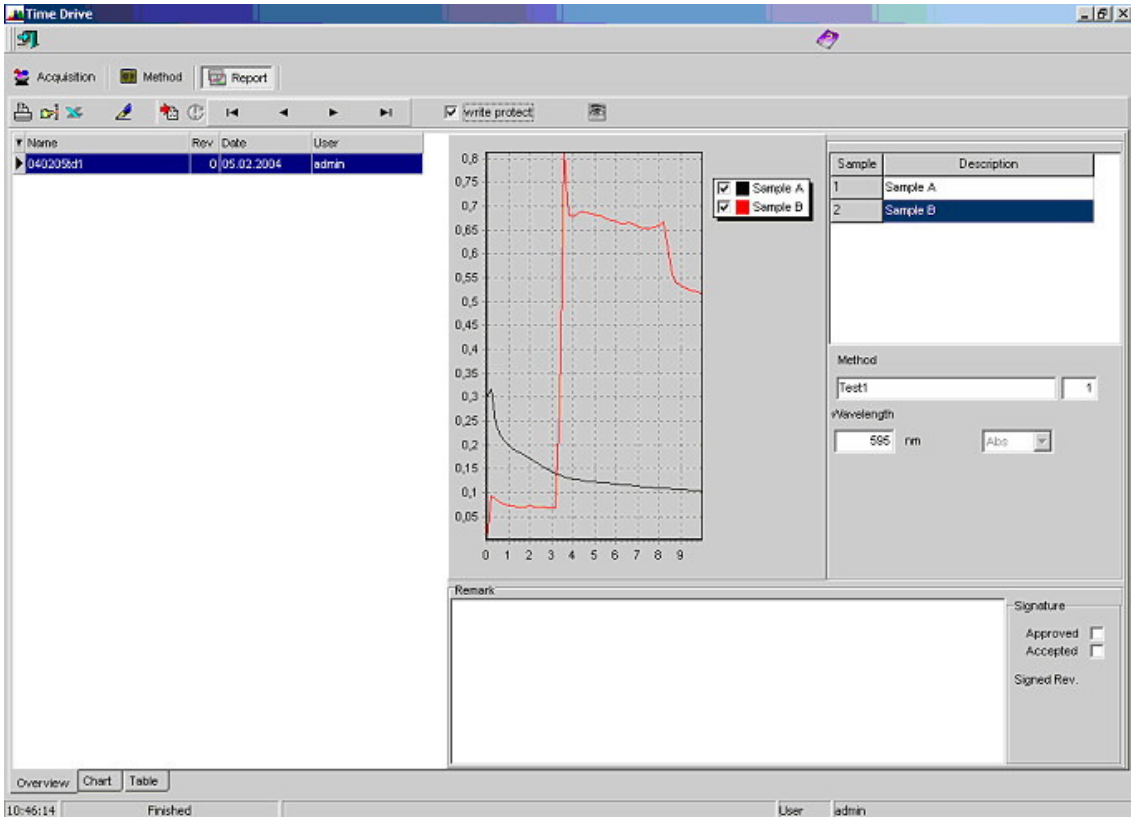


The calculation functions shown in the dialogue above are described in more detail in the section on *Calculation* within this document. Functions defined above will be included and stored with the method and thus used for any acquisition executed utilising that method.

2.4.3.3. The Report Screens in Time Drive

2.4.3.3.1. The "Overview" Report Screen

Click on the *Report* button in the upper left corner to open the *Report* window:



The display obtained is the "Overview" screen, clicking on the "Chart" tab will display the chart as the main item and this can be manipulated or edited as required.

The tabs for *Activity* and *Peak Detection* show a display in table form for the respective parameters

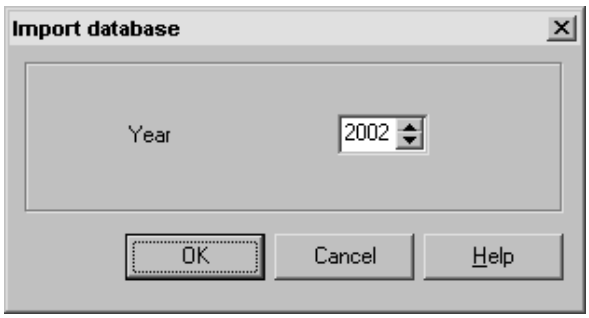
The left-hand window contains a list of all available reports, the right-hand window contains the results in the upper section and the main parameters for the measurement in the lower part. Each report can be viewed by scrolling through the left-hand list.

2.4.3.3.2. Printing

Click on the *Print* icon to obtain a print preview of the selected report, which will always contain all measurements. The report can be printed by clicking on the *Print* icon on the preview page.

2.4.3.3.3. Importing a report from the database

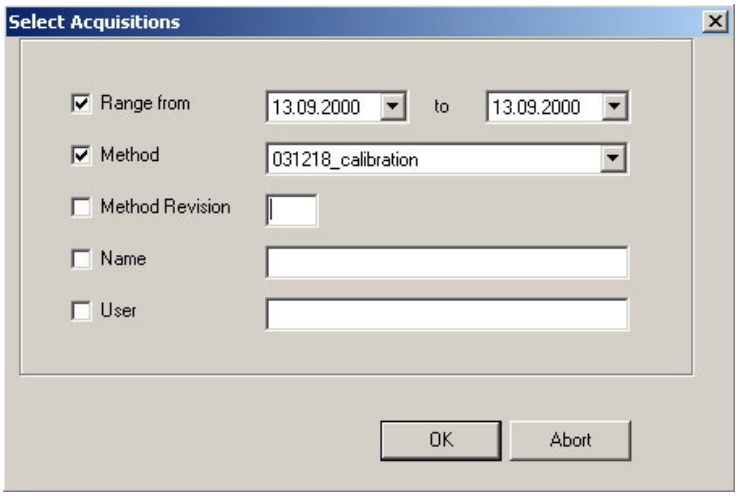
Click on the import icon to access earlier reports in the archived database. A dialogue window for selection of the database will be opened:



2.4.3.3.4. Filtering the report list

The report list in the left window will become very long with time and it may be necessary to filter the list so that only files of interest are shown to a user. This is carried out using the *Select Report* icon.

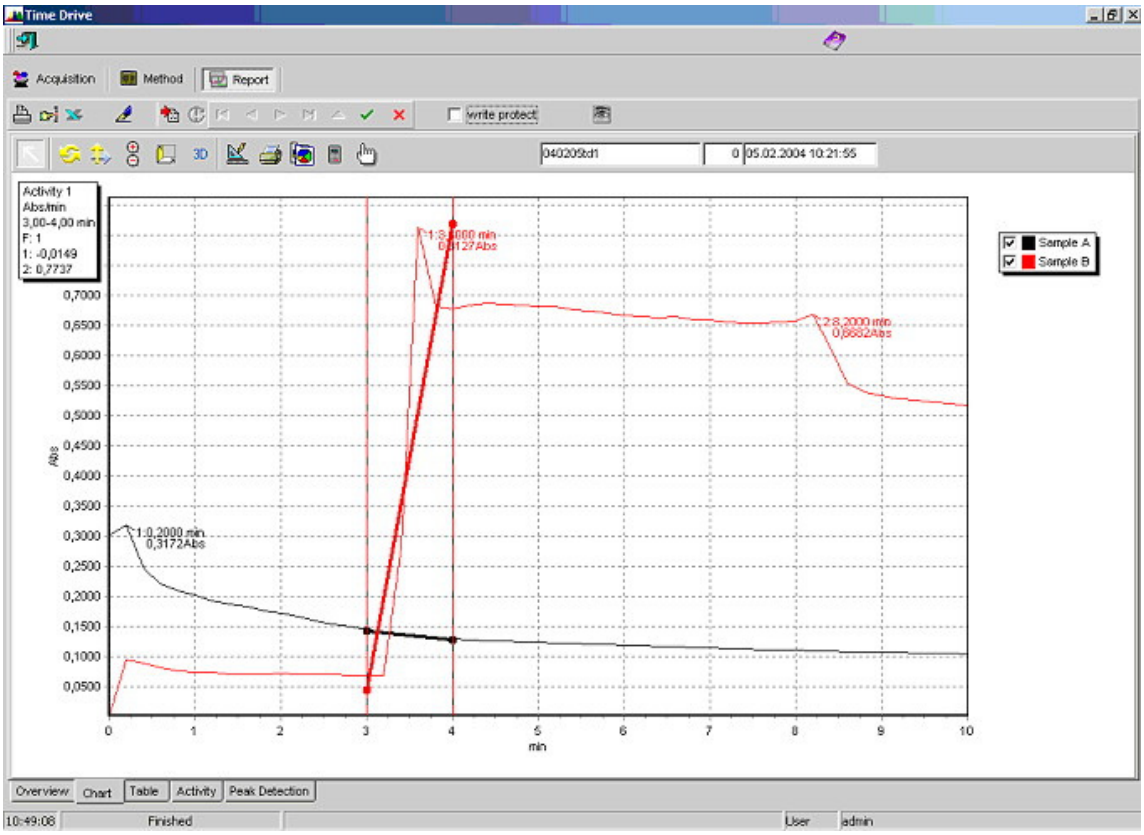
Click on the *Select Report* icon and a dialogue window appears, which allows selection of a view by date, method, user or name:



The appropriate checkboxes must be checked and, where applicable, either a date or name selected. Clicking on *OK* will cause only those reports which satisfy all selected criteria to be shown in the list of available reports.

2.4.3.3.5. The "Chart" Report Screen

Clicking on the "Chart" tab will open a new screen containing the curve in a form which can be edited:



To edit in cursor mode, uncheck the "write protect" checkbox first.

Navigation arrows are available to move between the various reports contained in the list without the need to return to the *Overview* screen.

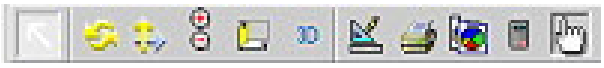
The name of the currently displayed curve set including the revision is shown in the box display immediately above the curve display.

In *Chart* mode a range of new functions is available to the user for manipulating the presentation and properties of the current curve.

Similar to the function "Peak Picking" in WL Scan, the new function "Time Picking" allows selecting the time (using the hand symbol). With a right mouse click the absorbance values can be selected at the cursor time position.
The manually selected list can be included into the document by selection the print option "Add peak detection to document". In this case a list including all selected values is inserted above the graphics.

2.4.3.3.6. "Chart" Report Screen Functions

A graphics toolbar is available within the *Chart report screen*:



The use of the icons in the graphics toolbar allow direct manual manipulation of the currently displayed chart. The function of the individual icons is described briefly below:

Shows position of values on X- and Y-axis and allows to manually pick peaks and to add, edit or delete comments.

Opens the calculation dialogue window.

Exports a curve to the *Windows clipboard* for further processing.

Prints the curve as a single sheet report. Formatting of the report is described in a separate section of this document dealing with curve format.

Opens the edit dialogue for formatting functions. See the separate section of this document dealing with curve format for more details.

Converts chart format to a 3D display. The icon functions as a toggle switch between a 2D and 3D display.

Click on this icon to control the depth of the 3D display using the mouse cursor. Clicking on this icon automatically converts the display format to 3D, return to the 2D display via the 3D icon button.

Double function icon allowing zooming of the complete curve.

Click on this icon to move the complete curve display using the mouse cursor. Clicking on this icon automatically converts the display format to 3D, return to the 2D display via the 3D icon button.

Click on this icon to rotate the complete curve display using the mouse cursor. Clicking on this icon automatically converts the display format to 3D, return to the 2D display via the 3D icon button.

Clicking on this icon will return the function of the mouse cursor to normal thus allowing use of the normal zooming functions etc. in 3D displays.

2.4.3.4. Calculations in Time Drive

The calculation modes for curves and activities are generally embedded in the method and are described above and in detail in the Calculation section.

Recalculation after, for example, changing a *Peak Detection* parameter is possible at any time by clicking on the Calculator icon followed by selection of the parameter within the dialogue window.

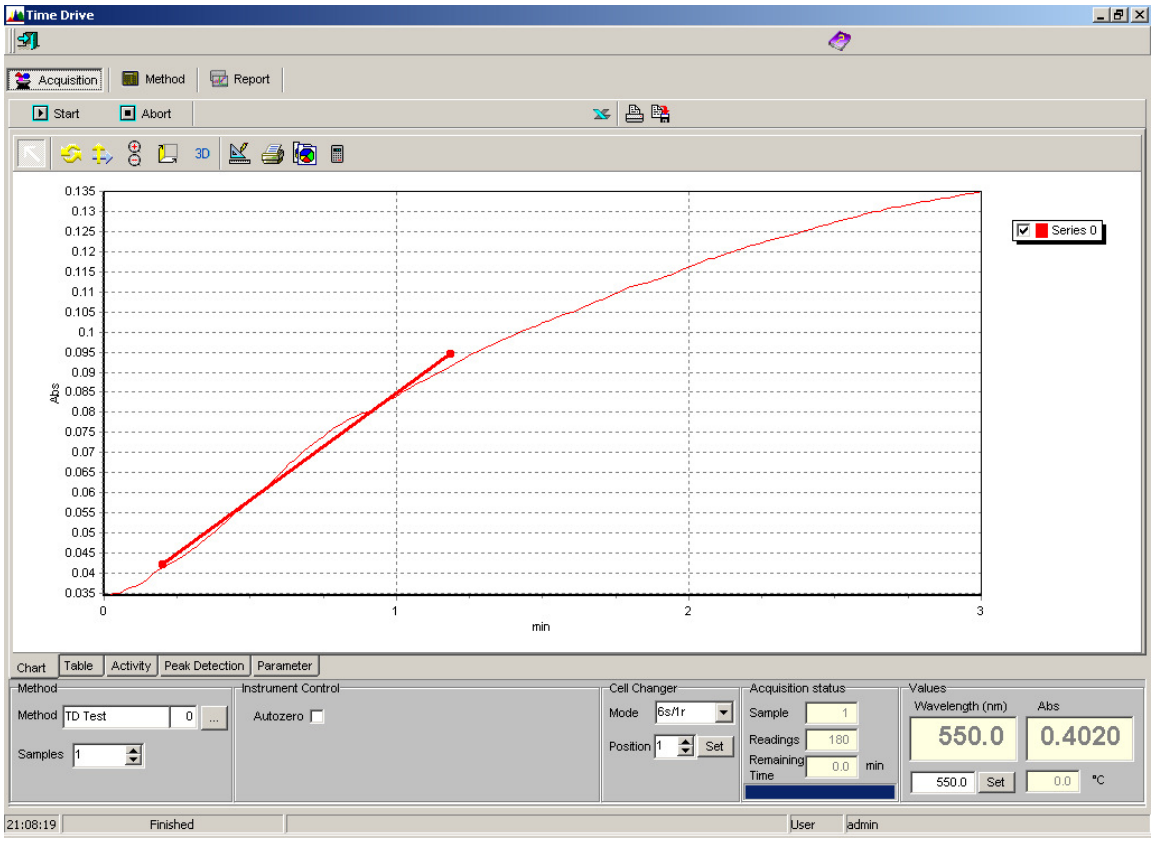
2.4.3.5. Time Drive Measurement Example

Measurement of a sample.

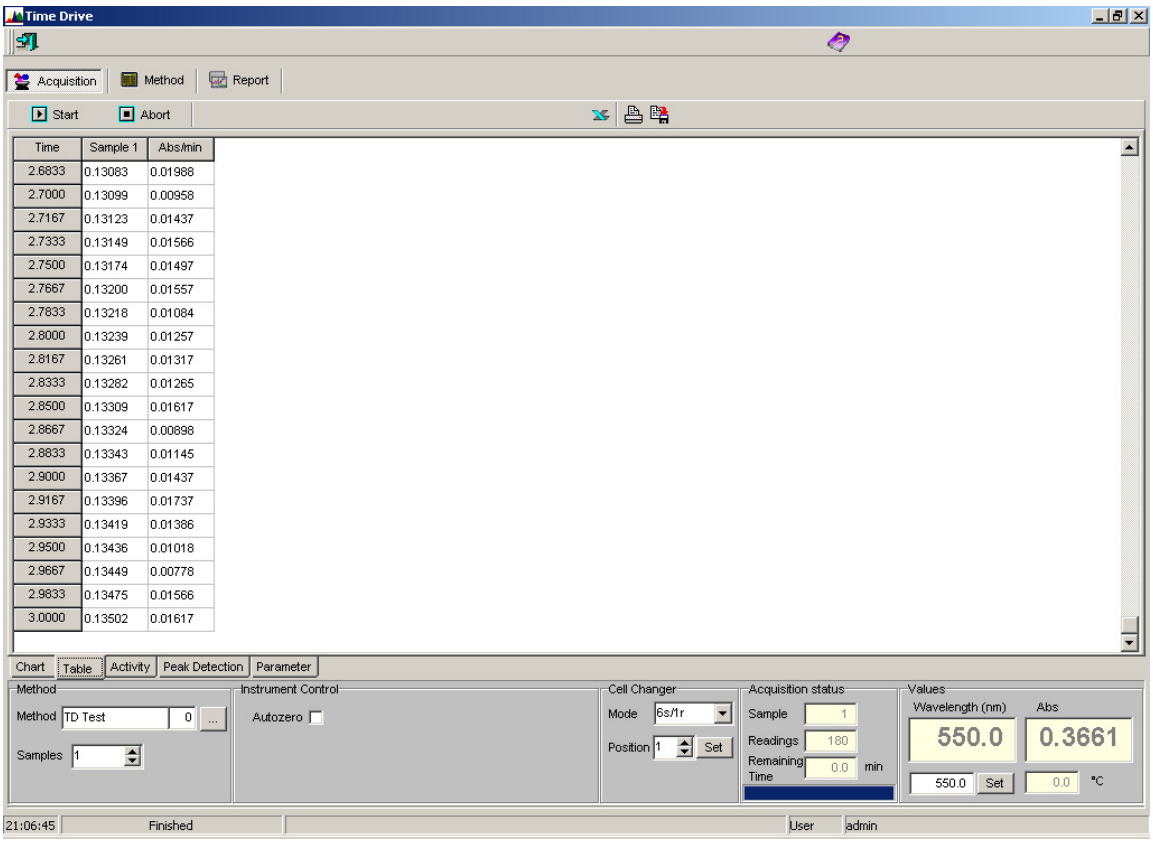
Select the method to be used and set the number of samples to 1.

Start the measurement by pressing the *Start* button and you will be prompted to insert the sample and click on *OK* to start the measurement. Insert the sample in the correct position and click on *OK*. The unit will now start to measure. The final windows will look like this:

The curve display is plotted during the acquisition and can be used to monitor the progress of the measurement. If the auto-calculation box has been checked, the regression line for the *Activity* calculation will be drawn immediately upon completion of the run.

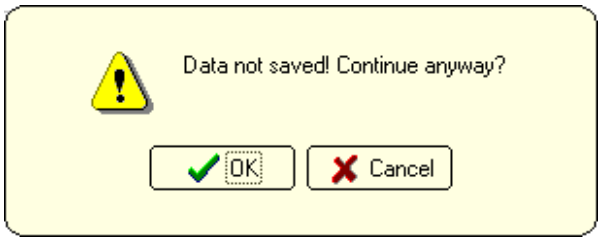


Various tab functions in the acquisition screen allow quick overviews of the results in table format (as shown below), activity etc.



Note: *If you have programmed more than one sample you will be prompted for the next sample after each sample has been measured. The final appearance of the screen remains unchanged.*

If you repeat the measurement you will always measure the selected number of samples (1 in our example) until you change the *Samples* parameter. The system will prompt if the previously run sample data has not been saved before starting a new run:



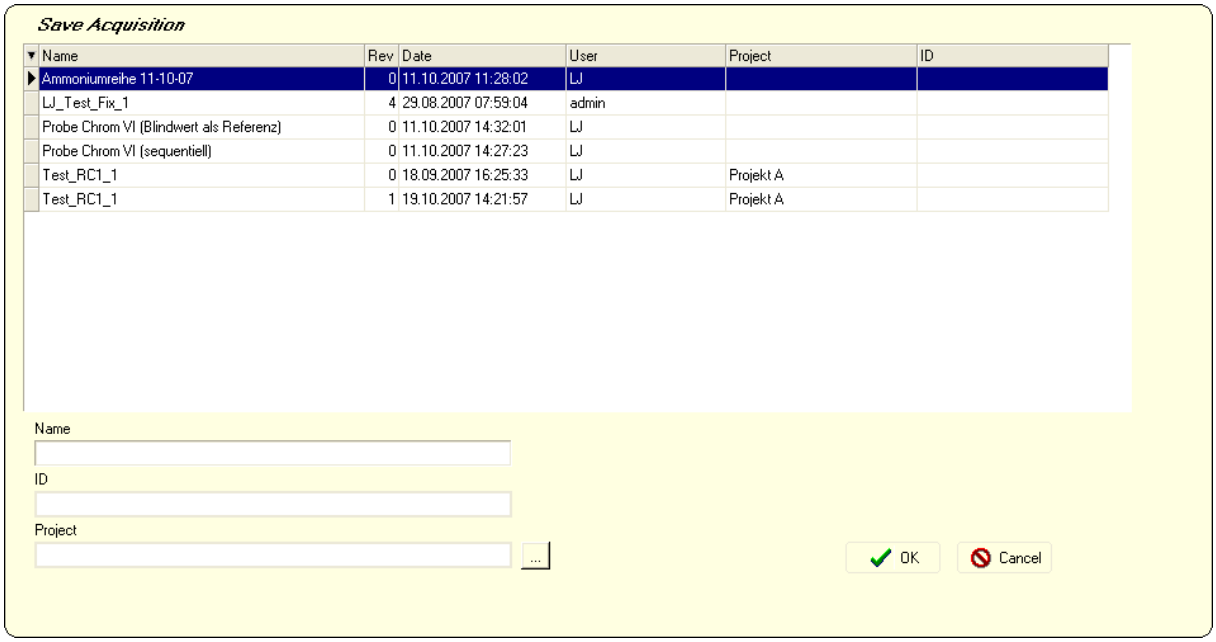
Click on *OK* to start the next acquisition run or on *Cancel* to return to the original data set.

Printing

Click on the *Print* icon to obtain a preview of the printed report, which will always contain all measurements. If the result is acceptable the report can be printed by clicking on the *Print* icon on the preview page.

Saving

Click on the *Save* icon and the system will prompt for a file name:



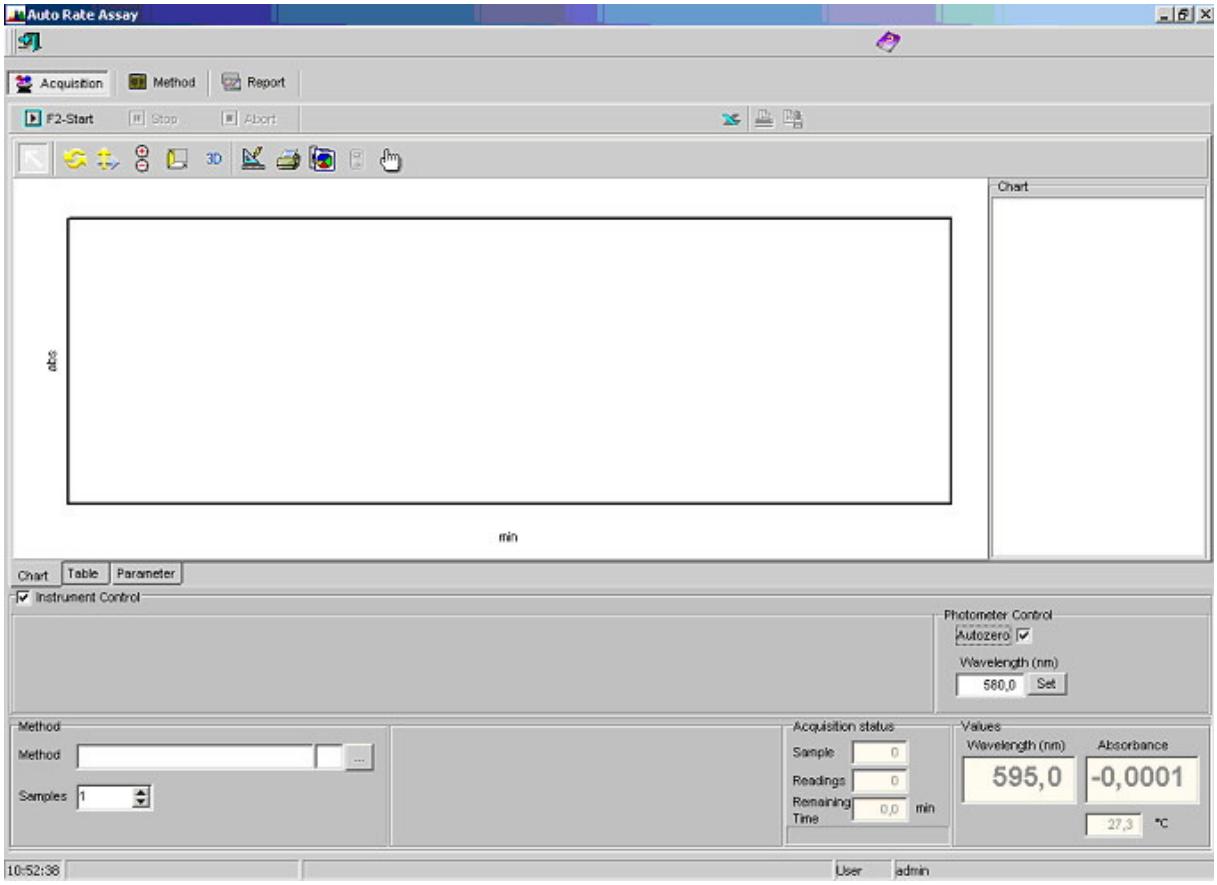
Enter the file name and click on *OK*.

2.4.4. Auto Rate Assay

The Autorate Assay mode is only possible in conjunction with an automatic cell changer. Operation is basically identical with that of Time Drive.

2.4.4.1. The Acquisition Screen in Autorate Assay

Select **"Autorate Assay"** from the main menu to obtain the following display:



This is the acquisition window from which all measurements are started. In this window the following parameters must be selected before starting a measurement:

- Method to be used for the acquisition. The method contains all parameters necessary for the execution of the measurement.
- Numbers of samples to be measured.
- *Autozero* at start of measurement.
- Load previous saved data from a report

2.4.4.1.1. Run parameters

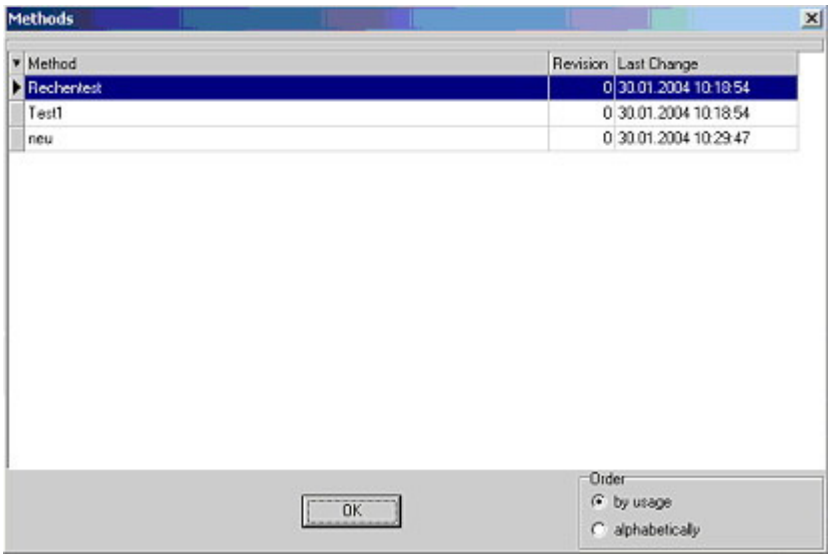
The run parameters are entered in the “Method” panel and in the “Photometer control” panel:

Samples Defines the number of samples to be analysed.

Checkbutton Press this button to accept the number of samples, the sample grid will also created.

Autozero Defines whether an autozero should be executed before starting a measurement.

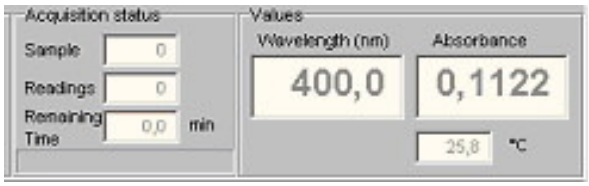
Method The method box contains the name of the method and, directly adjacent, the actual revision number of that method. The method is selected from a separate window which is opened by clicking on the button adjacent to the revision box:



This window contains a list of all available methods including all revisions of the method and the date of last modification. Selection is made by highlighting the required line and then clicking on *OK*.
The order of Methods may be displayed by usage or alphabetically.

Wavelength A certain wavelength may be chosen manually and set immediately in order to allow rapid monitoring of the unit.

2.4.4.1.2. System Status

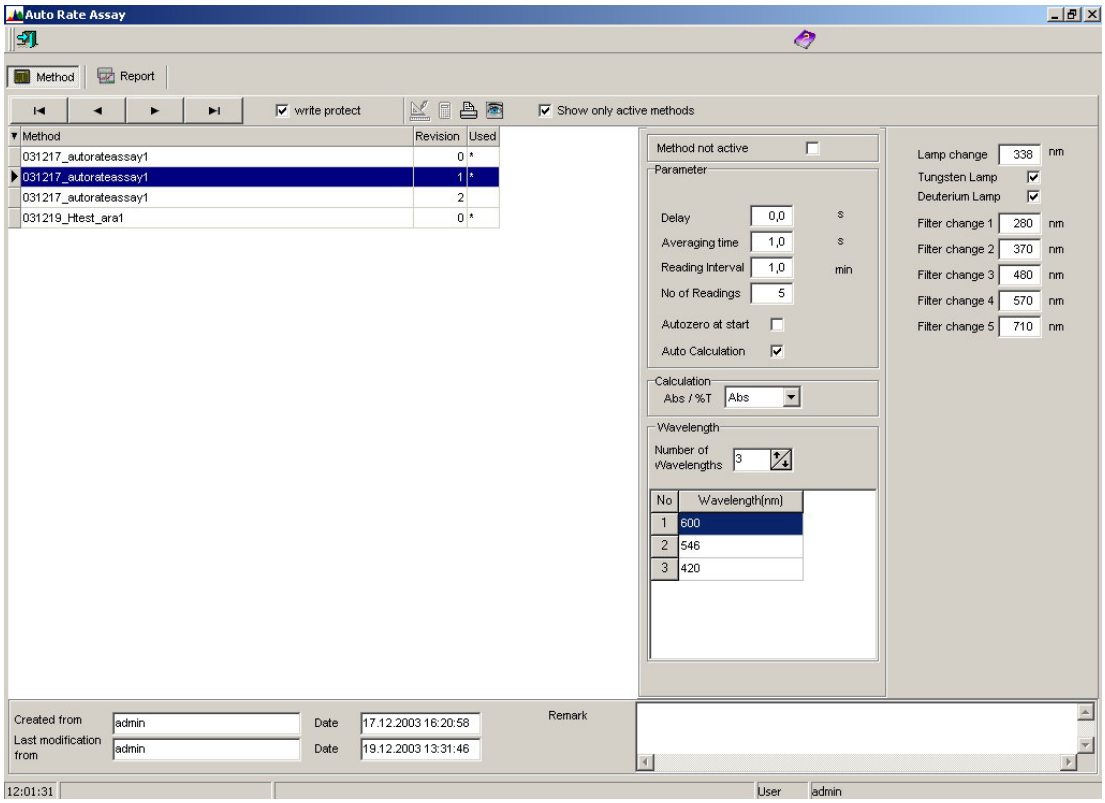


The lower right section of the display contains the actual status of the system and displays the following parameters:

- Current sample being measured.
- No. of Readings
- Remaining Time (also as progress bar)
- Actual wavelength.
- Actual absorbance value.
- Temperature (where applicable).

2.4.4.2. The Method in Autorate Assay

Click on the *Method* button in the upper left corner to open the *Method* window:



The left-hand window contains a list of all existing methods including revisions and an indication of whether they have been used already or not.

Caution: *If measurements have been used, the method will be locked and can no longer be changed. However, they can be used for later measurements or modified with revision control. Such methods are indicated by a " * " in the " used " column list.*

A new method can be created from within the method section by using the '+' button. In order to do this it is first necessary to uncheck the write-protect checkbox.

The system will first prompt for name under which the new method will be saved. Once this has been defined all other parameters can then be entered.

2.4.4.2.1. Acquisition parameters

Delay time The instrument will wait for the selected delay time after the MEASURE key is pressed to start the actual measurement.

Averaging time Defines the time the instrument uses to collect data for calculation of a mean value for one reading. A long averaging time is useful to reduce noise when measuring at high absorbance values.

Measure time Defines the actual duration of the measurement in minutes.

Sampling rate Defines the number of data points per minute for the measurement.

Autozero at start Defines whether an autozero is to be executed beforeeach sample run.

Auto Calculation If checked, the calculation for peak detection, smoothing etc. starts automatically after acquisition using the defined parameters.

Calculation mode Calculation and curve portrayal can be in either *Absorbance* or *Transmission* units.

Wavelength mode Defines the amount and the wavelengths to be used during measurement.

2.4.4.2.2. Common Parameters

The right-hand panel contains common parameters, which are required for every system and user method. They will be stored and recalled along with all other parameters.

Lamp change This parameter defines the lamp change wavelength. The deuterium lamp is used for all wavelengths below the lamp change wavelength. The tungsten halogen lamp is used for all wavelengths above the lamp change wavelength.

Tungsten lamp When checked, the tungsten lamp will be switched on and used according to the setting for the lamp change.

Deuterium lamp When checked, the deuterium lamp will be switched on and used according to the setting for the lamp change.

Filter change (1-5) This parameter defines the wavelength used to switch the filter.

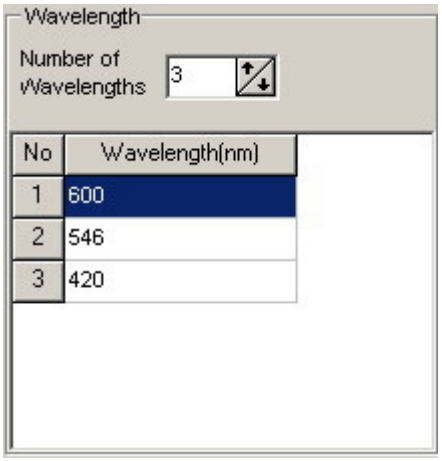
Bandwidth Selects the spectral bandwidth of the spectrophotometer.

Cell changer Defines the operating mode of the cell changer (if fitted).

2.4.4.2.3. Calculation

The calculation selection permits definition of the mode of calculation to be used. The user can select between either absorbance or transmission.

2.4.4.2.4. Wavelength



A maximum of six different wavelengths may be chosen. The λ of the wavelengths can be defined in the rows below.

2.4.4.2.5. Curve Parameters in the Auto Rate Assay Method

Opens an edit dialogue for defining curve parameters and related formatting.

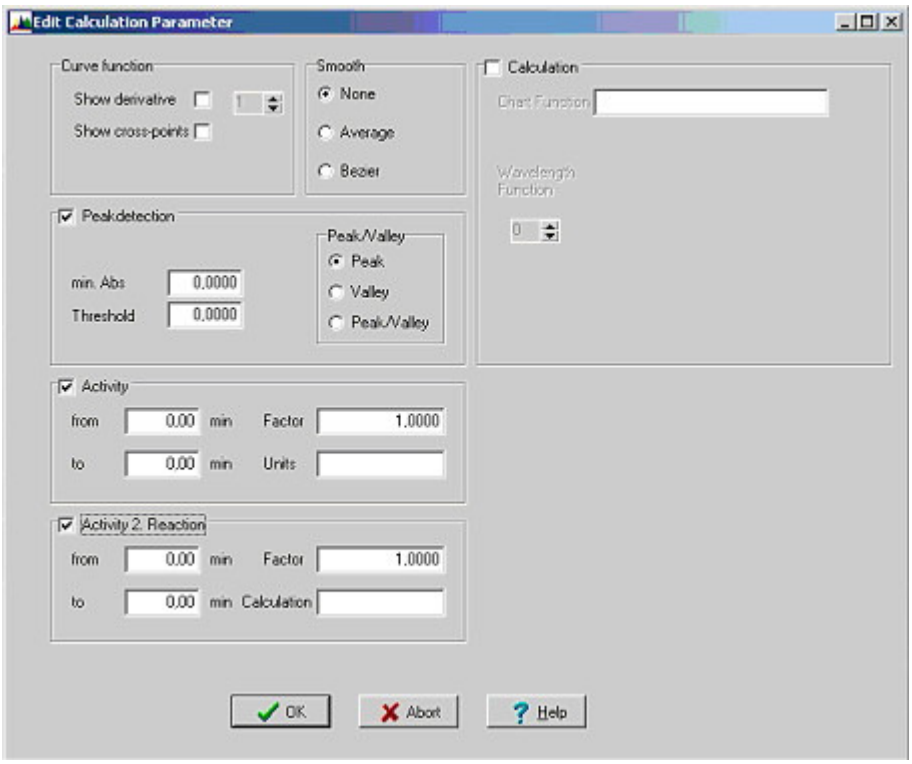
In *Auto Rate Assay* the curve parameters can be linked to a method and then define the appearance and properties of the curve such as colours, overlay format, scaling etc.

Functions defined here will be included and stored with the method and thus used for any acquisition executed utilising that method.

Formatting options using this function are described in a separate section in this document.

2.4.4.2.6. Calculation Parameters in the Auto Rate Assay Method

Click on this icon to open the calculation dialogue window for the method:

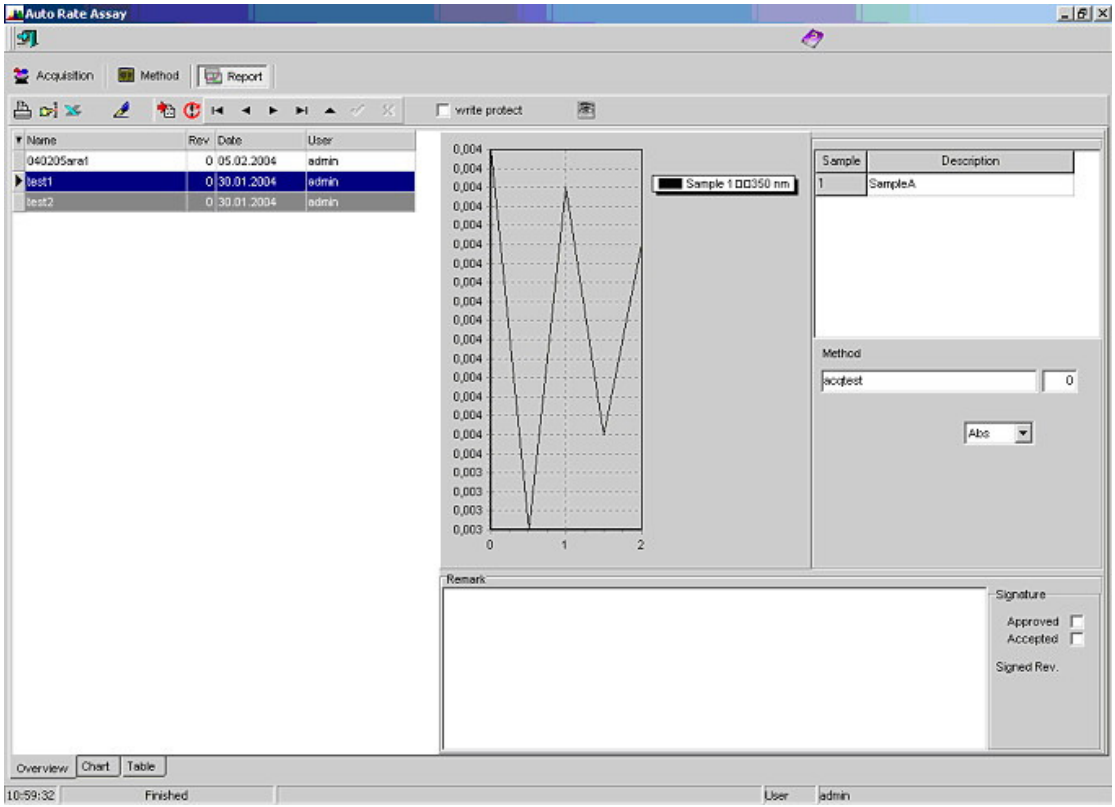


The calculation functions shown in the dialogue above are described in more detail in the section on Calculation within this document. Functions defined above will be included and stored with the method and thus used for any acquisition executed utilising that method.

2.4.4.3. The Report Screens in Autorate Assay

2.4.4.3.1. The "Overview" Report Screen

Click on the *Report* button in the upper left corner to open the *Report* window:



The display obtained is the "Overview" screen, clicking on the "Chart" tab will display the chart as the main item which can be manipulated or edited as required.

The tabs for *Activity* and *Peak Detection* show a display in table form for the respective parameters

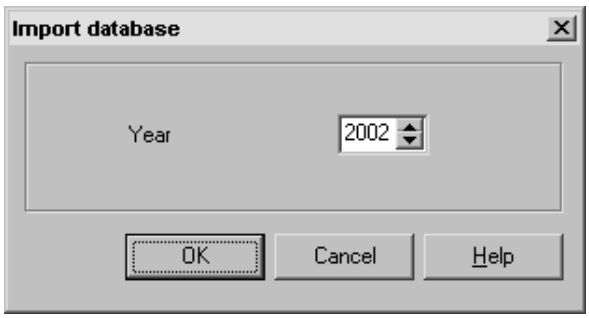
The left-hand window contains a list of all available reports, the right-hand window contains the results in the upper section and the main parameters for the measurement in the lower part. Each report can be viewed by scrolling through the left-hand list.

2.4.4.3.2. Printing

Click on the *Print* icon to obtain a print preview of the selected report, which will always contain all measurements. The report can be printed by clicking on the *Print* icon on the preview page.

2.4.4.3.3. Importing a report from the database

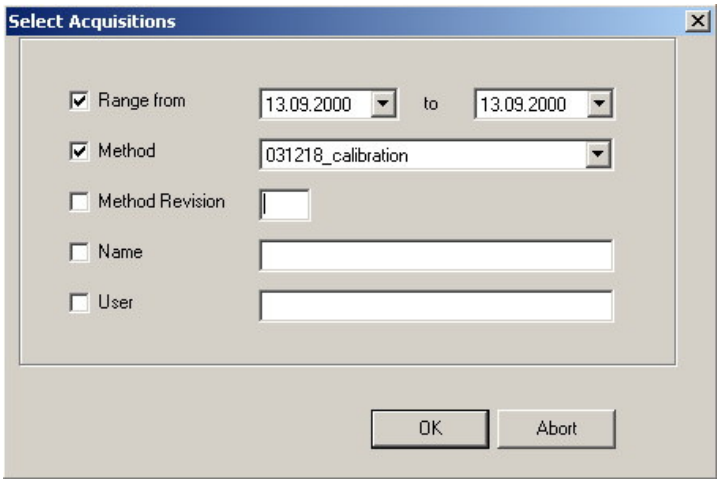
Click on the import icon to access earlier reports in the archived database. A dialogue window for selection of the database will be opened:



2.4.4.3.4. Filtering the report list

The report list in the left window will become very long with time and it may be necessary to filter the list so that only files of interest are shown to a user. This is carried out using the *Select Report* icon.

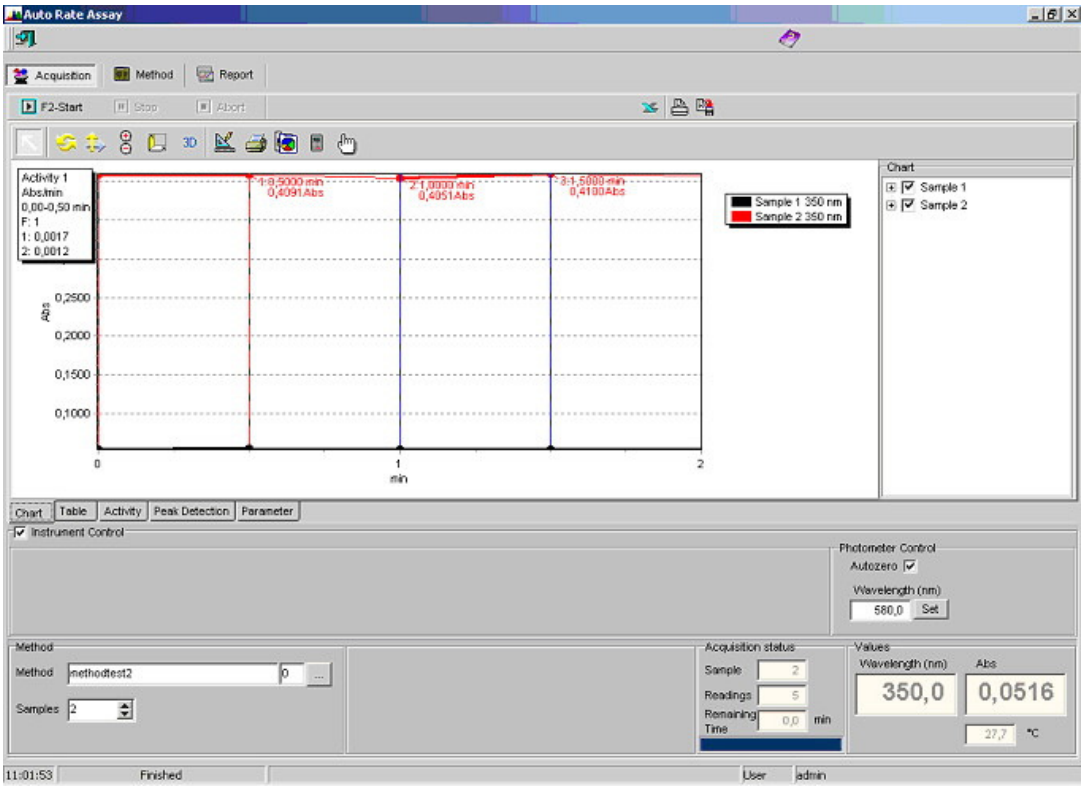
Click on the *Select Report* icon and a dialogue window appears, which allows selection of a view by date, method, user or name:



The appropriate checkboxes must be checked and, where applicable, either a date or name selected. Clicking on *OK* will show only those reports which match with selected criteria shown in the list of available reports.

2.4.4.3.5. The "Chart" Report Screen

Clicking on the "Chart" tab will open a new screen containing the curve in a form which can be edited:



Navigation arrows are available to move between the various reports contained in the list without the need to return to the *Overview* screen.

The name of the currently displayed curve set including the revision is shown in the box display immediately above the curve display.

In *Chart* mode a range of new functions is available to the user for manipulating the presentation and properties of the current curve.

Similar to the function "Peak Picking" in WL Scan, the new function "Time Picking" allows selecting the time (using the hand symbol). With a right mouse click the absorbance values can be selected at the cursor time position.
The manually selected list can be included into the document by selection the print option "Add peak detection to document". In this case a list including all selected values is inserted above the graphics.

2.4.4.3.6. "Chart" Report Screen Functions

A graphics toolbar is available within the *Chart report screen*:

The use of the icons in the graphics toolbar allow direct manual manipulation of the currently displayed chart. The function of the individual icons is described briefly below:

Shows position of values on X- and Y-axis and allows to manually pick peaks and to add, edit or delete comments.

Opens the calculation dialogue window.

Exports a curve to the *Windows clipboard* for further processing.

Prints the curve as a single sheet report. Formatting of the report is described in a separate section of this document dealing with curve format.

Opens the edit dialogue for formatting functions. See the separate section of this document dealing with curve format for more details.

Converts chart format to a 3D display. The icon functions as a toggle switch between a 2D and 3D display.

Click on this icon to control the depth of the 3D display using the mouse cursor. Clicking on this icon automatically converts the display format to 3D, return to the 2D display via the 3D icon button.

Double function icon allowing zooming of the complete curve.

Click on this icon to move the complete curve display using the mouse cursor. Clicking on this icon automatically converts the display format to 3D, return to the 2D display via the 3D icon button.

Click on this icon to rotate the complete curve display using the mouse cursor. Clicking on this icon automatically converts the display format to 3D, return to the 2D display via the 3D icon button.

Clicking on this icon will return the function of the mouse cursor to normal thus allowing use of the normal zooming functions etc. in 3D displays.

2.4.4.4. Calculations in Autorate Assay

The calculation modes for curves and activities are generally embedded in the method and are described above and in detail in the Calculation section.

Recalculation after, for example, changing a *Peak Detection* parameter is possible at any time by clicking on the *Calculator* icon followed by selection of the parameter within the dialogue window.

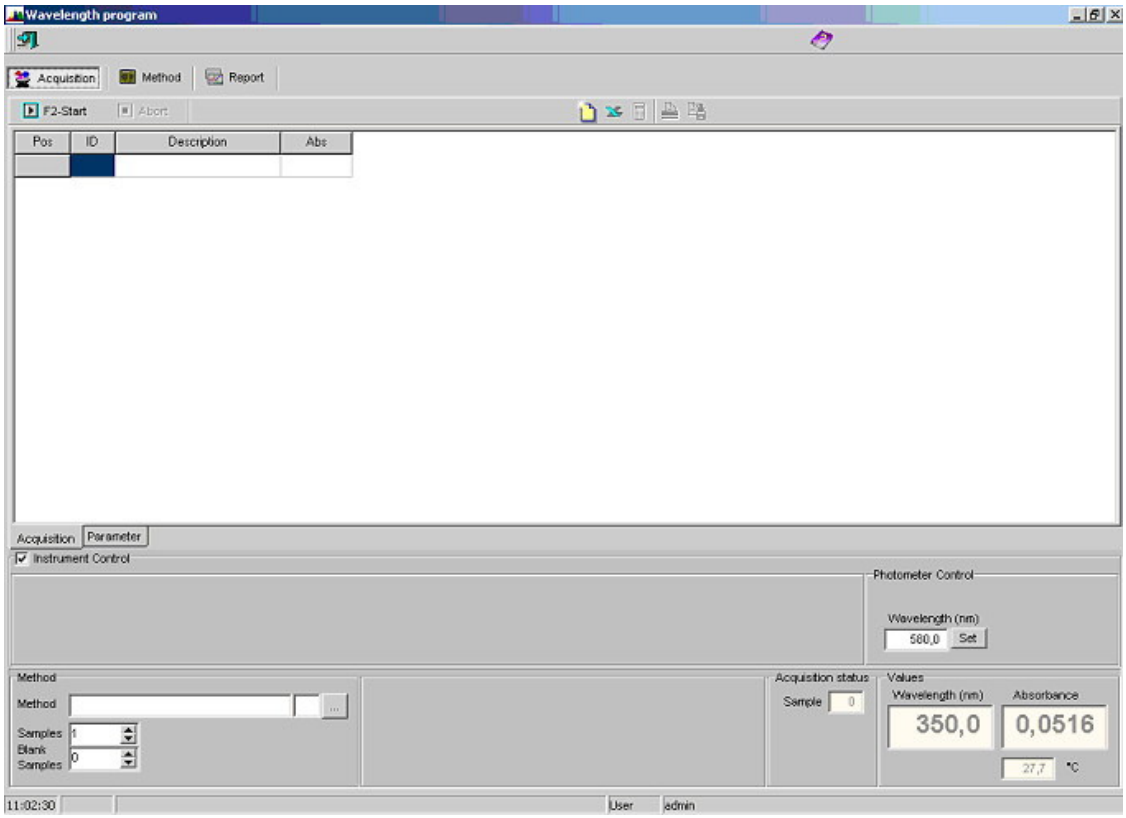
2.4.5. Wavelength Program

Wavelength Program mode permits measurements at different wavelengths and also calculations such as wavelength ratios to be made automatically for a set of samples.

The first samples measured can be defined as *Blanks* and the values of these samples will be averaged and then subtracted from each wavelength measurement of that particular sample.

2.4.5.1. The Acquisition Screen in Wavelength Program

Select **"Wavelength Program"** from the main menu to obtain the following display:

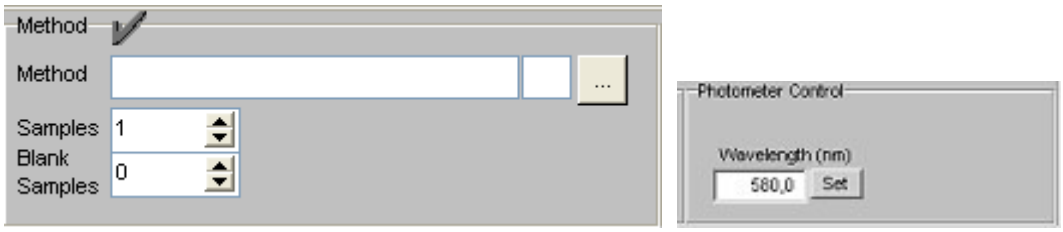


This is the acquisition window from which all measurements are started. In this window the following parameters must be selected before starting a measurement:

- Method to be used for the acquisition. The method contains all parameters necessary for the execution of the measurement.
- Numbers of samples to be measured.
- Number of blank samples, measured as the first samples.
- *Autozero* at start of measurement.

2.4.5.1.1. Run parameters

The run parameters are entered in the “Method” panel and in the “Photometer control” panel:

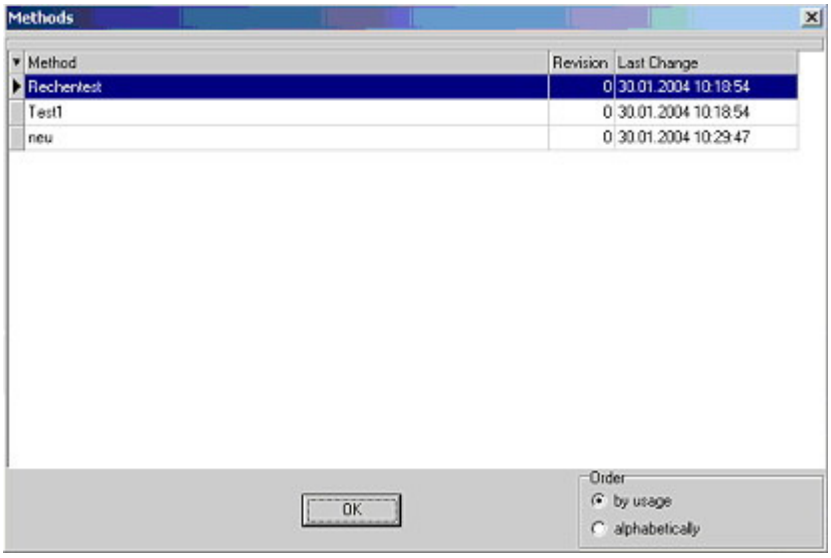


Samples Defines the number of samples to be analysed.

Checkbutton Press this button to accept the number of samples, the sample grid will also created.

Blank Samples Defines the number of blank samples to be measured, blank samples are always expected at the start of a run. The value of the measured blank is subtracted from the actual measured value of the sample prior to calculation of concentration etc. If more than one blank is defined then the system calculates the average blank value for the blanks and then subtracts this from the actual measured sample values.

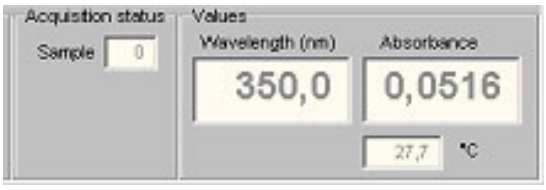
Method The method box contains the name of the method and, directly adjacent, the actual revision number of that method. The method is selected from a separate window which is opened by clicking on the button adjacent to the revision box:



This window contains a list of all available methods including all revisions of the method and the date of last modification. Selection is made by highlighting the required line and then clicking on *OK*.
The order of Methods may be displayed by usage or alphabetically.

Wavelength A certain wavelength may be chosen manually and set immediately in order to allow rapid monitoring of the unit.

2.4.5.1.2. System Status

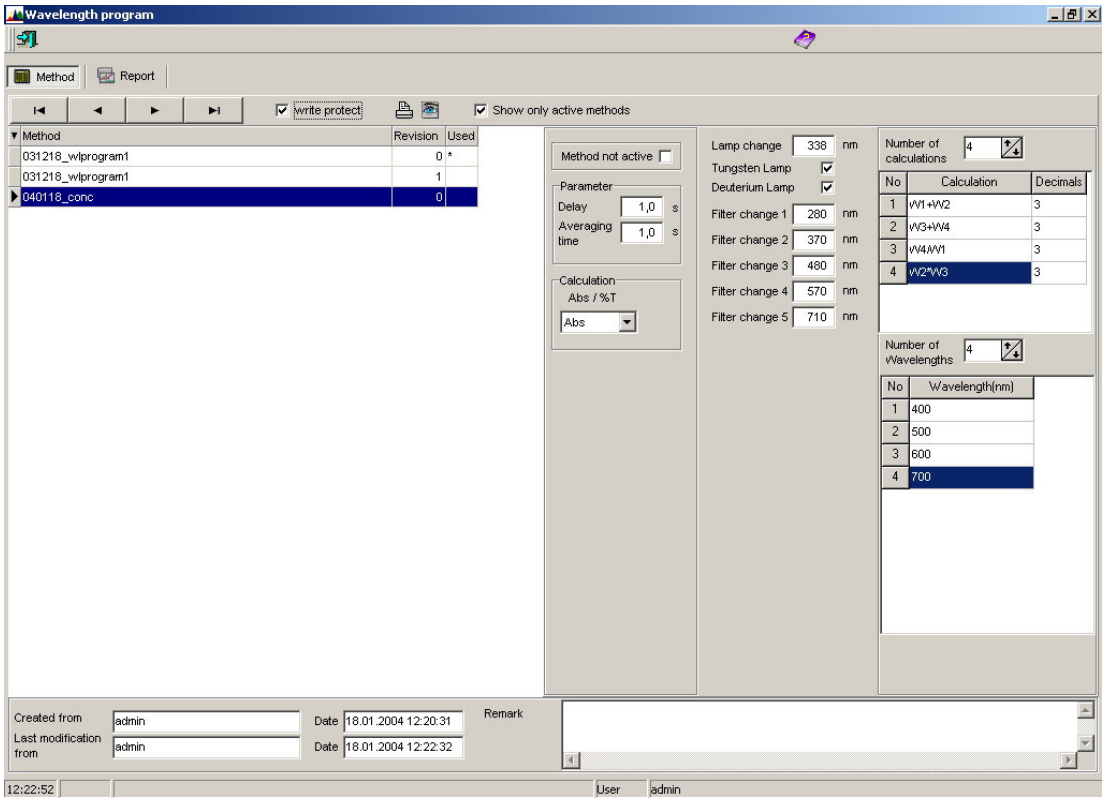


The lower right section of the display contains the actual status of the system and displays the following parameters:

- Current sample being measured.
- Actual wavelength.
- Actual absorbance value.
- Temperature (where applicable).

2.4.5.2. The Method in Wavelength Program

Click on the *Method* button in the upper left corner to open the *Method* window:



The left-hand window contains a list of all existing methods including revisions and an indication of whether they have been used already or not.

Caution: *If measurements have been used, the method will be locked and can no longer be changed. However, they can be used for later measurements or modified with revision control. Such methods are indicated by a " * " in the " used " column list.*

A new method can be created from within the method section by using the '+' button. In order to do this it is necessary to uncheck the write-protect checkbox.

The system will first prompt for name under which the new method will be saved. Once this has been defined all other parameters can then be entered.

2.4.5.2.1. Acquisition parameters

Delay time The instrument will wait for the selected delay time after the MEASURE key is pressed to start the actual measurement.

Averaging time Defines the time the instrument uses to collect data for calculation of a mean value for one reading. A long averaging time is useful to reduce noise when measuring at high absorbance values.

2.4.5.2.2. Common parameters

The right-hand panel contains common and calculations parameters, which are required for every system and user method. They will be stored and recalled along with all other parameters:

Lamp change This parameter defines the lamp change wavelength. The deuterium lamp is used for all wavelengths below the lamp change wavelength. The tungsten halogen lamp is used for all wavelengths above the lamp change wavelength.

Tungsten lamp When checked, the tungsten lamp will be switched on and used according to the setting for the lamp change.

Deuterium lamp When checked, the deuterium lamp will be switched on and used according to the setting for the lamp change.

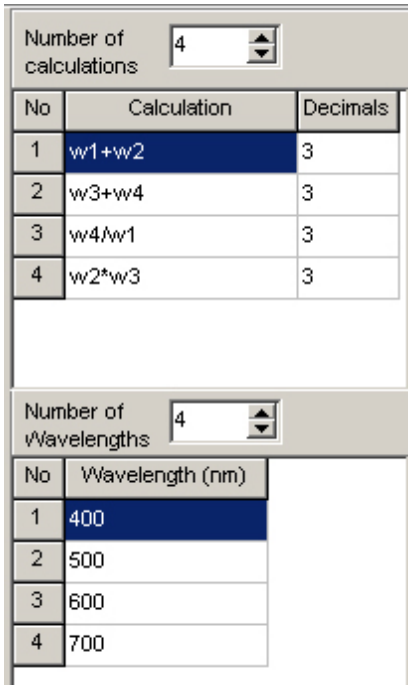
Filter change (1-5) This parameter defines the wavelength used to switch the filter.

Bandwidth Selects the spectral bandwidth of the spectrophotometer.

Cell changer Defines the operating mode of the cell changer (if fitted).

2.4.5.2.3. Wavelength Program calculations

The right section of the method screen allows definition of the wavelengths to be used and also the calculation modes:



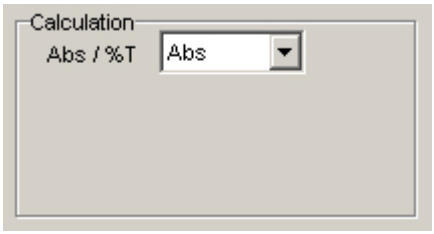
The required number of both calculations and wavelengths to be used must first be defined using the two spin boxes at the top of each entry window. This definition will open the appropriate number of lines where the actual values can be entered directly:

Calculation: Wavelengths are defined for calculation purposes as W(n) or w(n) respectively, where (n) corresponds to actual number for a given wavelength as shown in the lower window. In the example above the following calculations will be performed:

1.	Wavelength number 1, e.g. at 400 nm is added to	Wavelength 2.
2.	Wavelength number 3, e.g. at 600 nm, is added to	Wavelength 4
3.	Wavelength number 4, e.g. at 700 nm is divided by	Wavelength 1
4.	Wavelength number 2, e.g. at 500 nm, is multiplied by	Wavelength 3

Decimals: The number of decimal places to be used for the calculation can also be defined. This number should generally be consistent with the actual measured result, e.g. by measurements to 4 decimal places, selection of a much higher number for the calculation result will not increase the accuracy of a measurement or result and could produce rounding errors.

2.4.5.2.4. Calculation



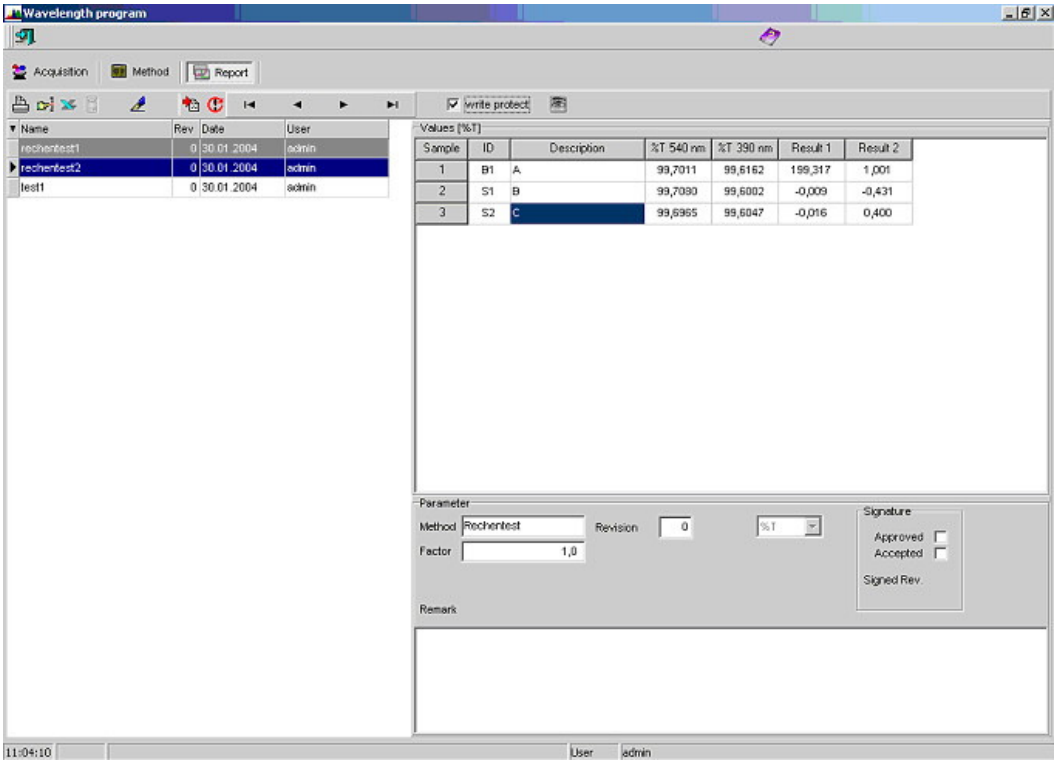
The calculation selection permits definition of the mode of calculation to be used, the user can select between either absorbance or transmission.

2.4.5.2.5. Audit Trail in Wavelength Program Method

Click on the *Audit Trail* icon to view the audit trail window for a method.

2.4.5.3. The Report Screen in Wavelength Program

Click on the *Report* button in the upper left corner to open the *Report* window:



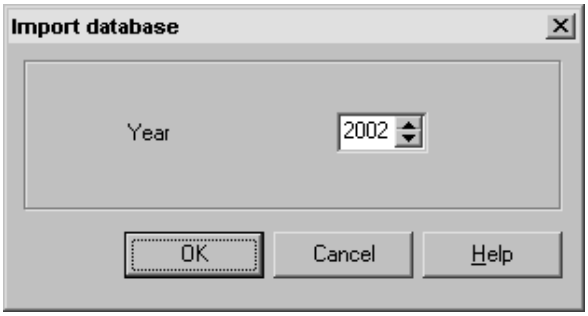
The left-hand window contains a list of all available reports, the right-hand window contains the results in the upper section and the main parameters for the measurement in the lower part. Each report can be viewed by scrolling through the left-hand list. Data can be viewed in the right-hand window by scrolling across the table using the mouse.

2.4.5.3.1. Printing

Click on the *Print* icon to obtain a print preview of the selected report, which will always contain all measurements. The report can be printed by clicking on the *Print* icon on the preview page.

2.4.5.3.2. Importing a report from the database

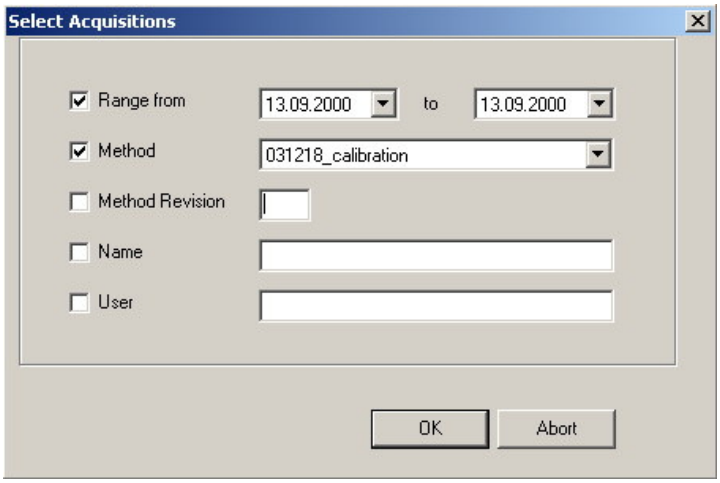
Click on the import icon to access earlier reports in the extracted database. A dialogue window for selection of the database will be opened:



2.4.5.3.3. Filtering the report list

The report list in the left window will become very long with time and it may be necessary to filter the list, so that only files of interest are shown to a user, using the *Select Report* icon:

Click on the *Select Report* icon and a dialogue window appears, which allows selection of a view by date, method, user or name:



The appropriate checkbox must be checked and, where applicable, either a date or name selected. Clicking on *OK* will cause only those reports which match with selected criteria shown in the list of available reports.

2.4.5.3.4. Audit Trail in Wavelength Program Report

Click on the *Audit Trail* icon to view the audit trail window for a report:

2.4.5.4. Calculations in Wavelength Program

Wavelength Program contains, alongside the basic wavelength calculations described above, two additional calculation methods for the final result determination:

- Blank
- Factor

In *Wavelength Program* the *Blank* and *Factor* calculations can be executed automatically without the need to create a calibration file:

Blank The measured values for sample blank at each wavelength is subtracted from the measured value of each measured sample at the same wavelength.

Factor The actual value obtained from the measurement is always multiplied by the factor parameter. This is accessible by clicking on the *Parameter* tab in the acquisition screen.

The actual calculation is based on the following formula at any given wavelength:

$$RW = F * (VM_{sample} - VM_{blank})$$

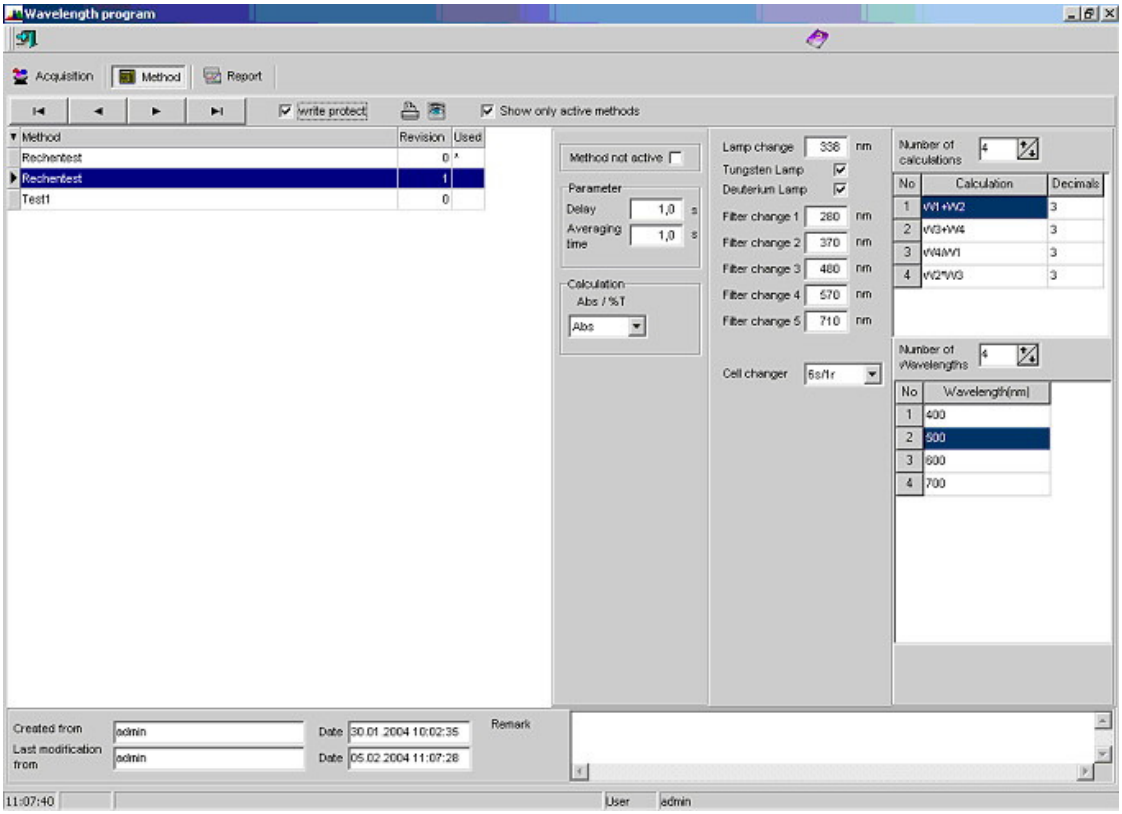
Where RW = Result for wavelength W, F = Factor and VM represents the measured values obtained for sample and blank respectively. The value RW is then used for the defined calculations for the individual wavelengths.

Recalculation after, for example, changing the factor value is possible at any time by clicking on the *Calculator* icon **before** the data has been saved..

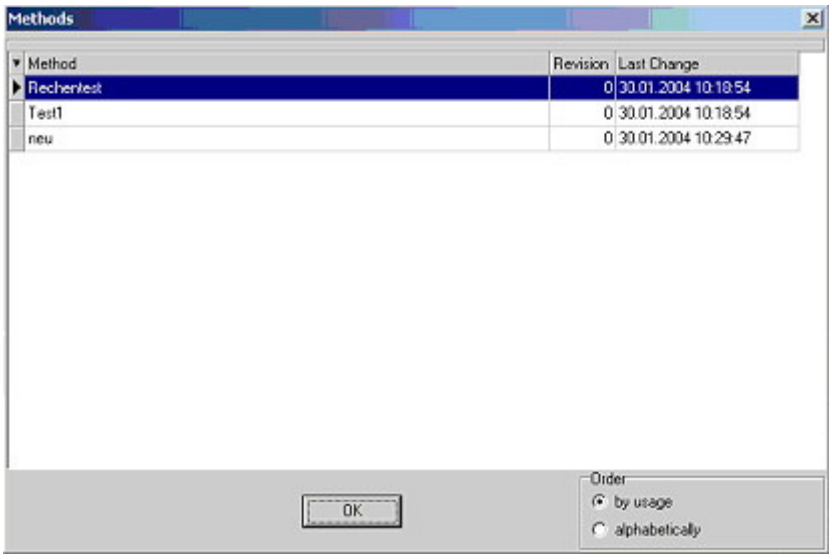
2.4.5.5. Wavelength Program Measurement Example

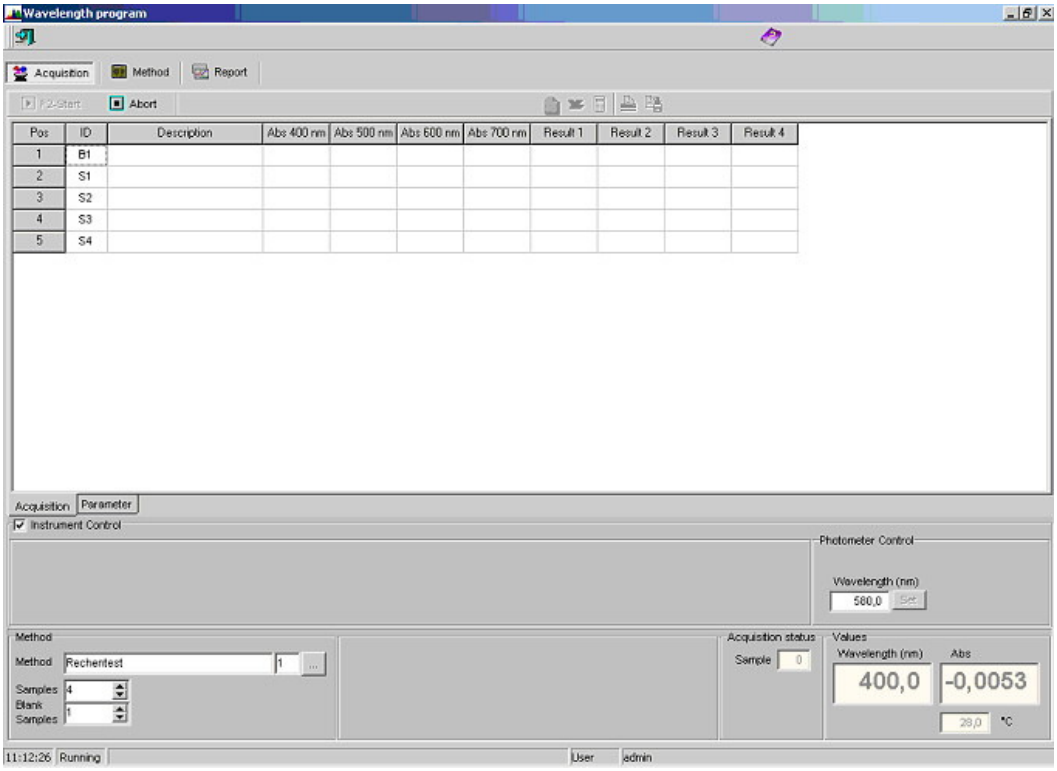
Wavelength Program measurement of 4 samples using an optional automatic 6+6 cell changer. Four wavelengths are used (400, 500, 600 and 700 nm). The first sample is a Blank.

Define the method to be used:

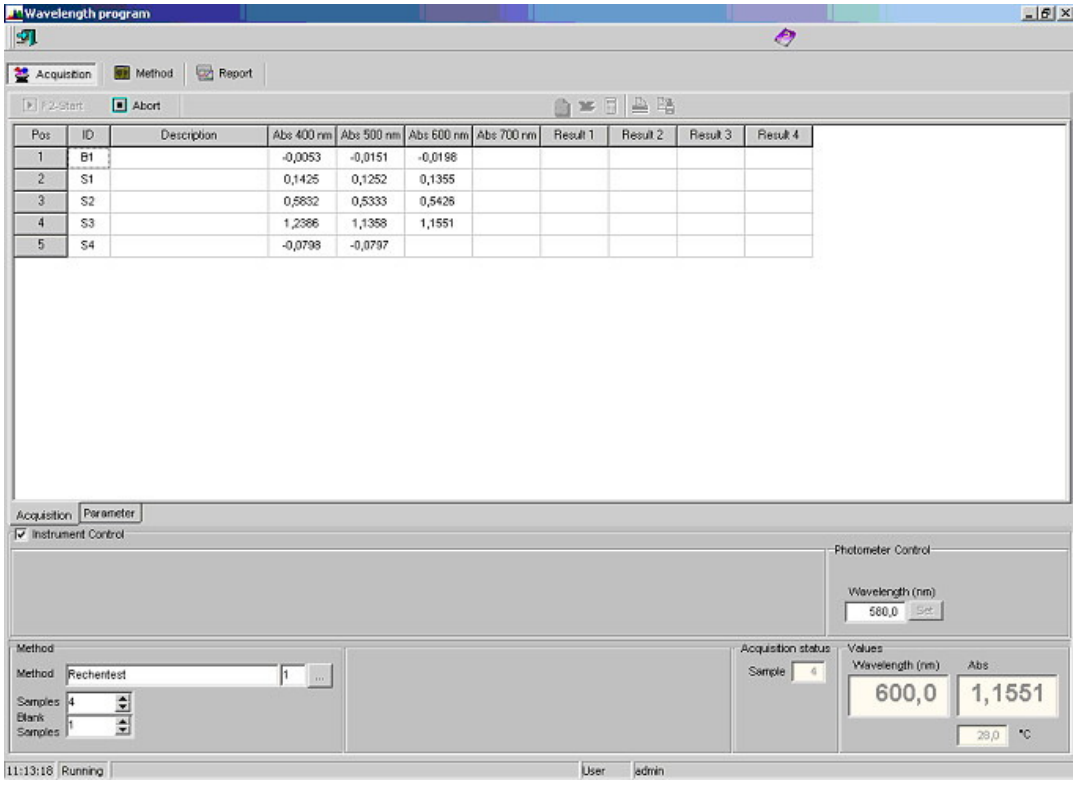


Click on the *Acquisition* tab in the upper left corner and select a method by clicking on the button next to the method window in the lower left of the screen:

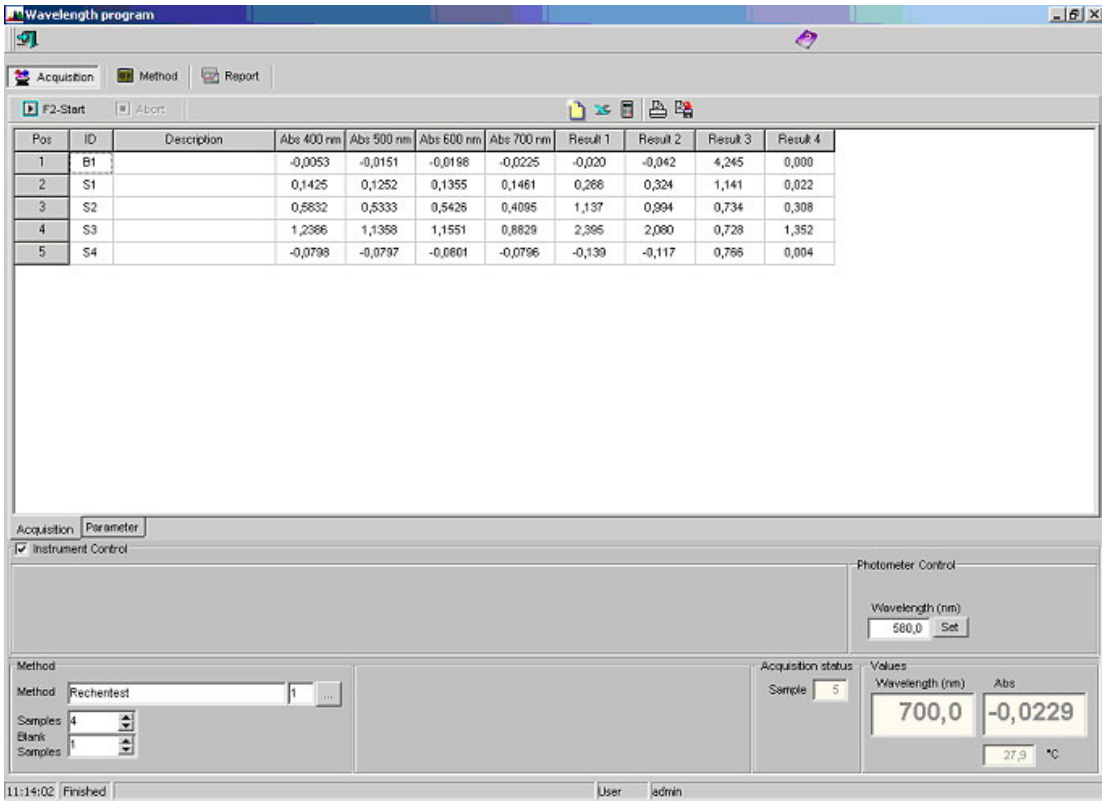




Set the number of samples to 4 and the Blank Samples to 1. Enter descriptions if required and insert the *Blank* sample in position 1 in the cell changer and the four samples in positions 2 to 5. Start the measurement by pressing the *Start* button. The measured values will be displayed during acquisition:

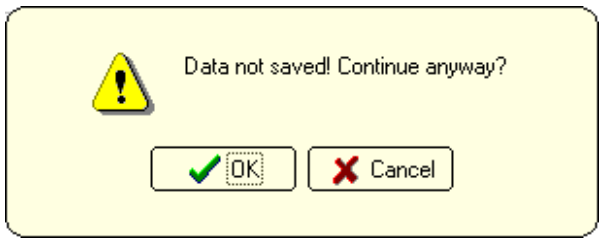


The final window will look like this:



Note: *If you are not using a cell changer, you will be prompted for the next sample after each sample has been measured. The final appearance of the screen remains unchanged.*

If you repeat the measurement you will always measure the selected number of samples (3 in our example) until you change the *Samples* parameter. The system will prompt if the previously run sample data has not been saved before starting a new run:



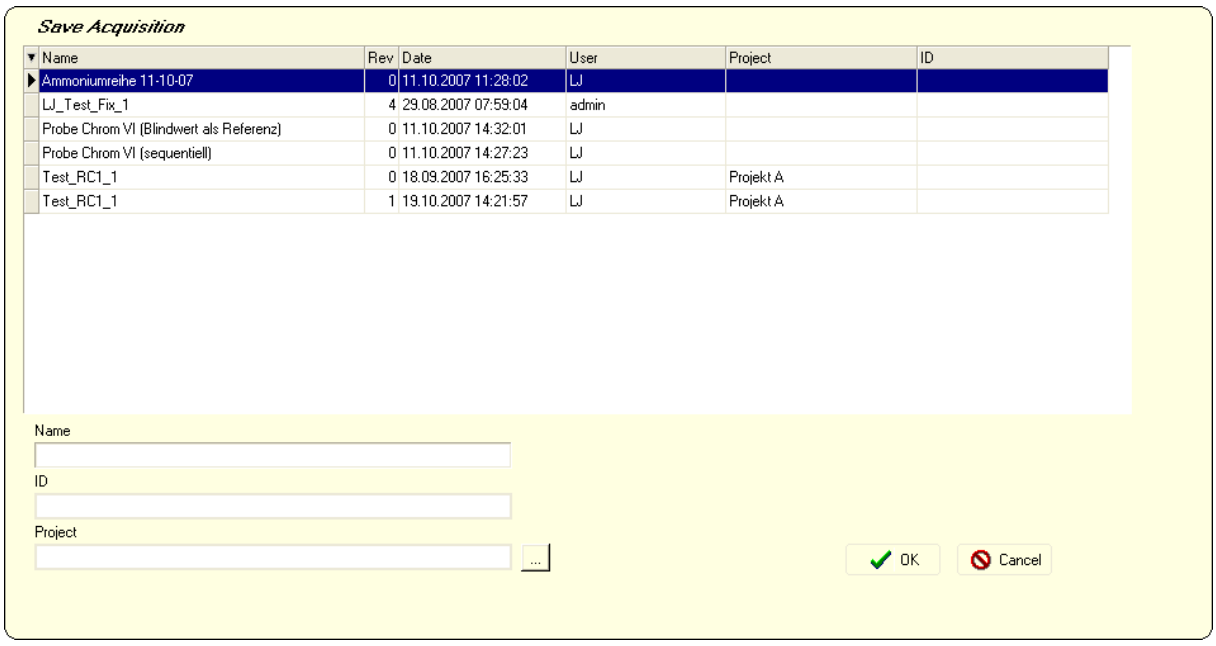
Click on *OK* to start the next acquisition run or on *Cancel* to return to the original data set.

Printing

Click on the *Print* icon to obtain a preview of the printed report, which will always contain all measurements. If the result is acceptable the report can be printed by clicking on the *Print* icon on the preview page.

Saving

Click on the *Save* icon and the system will prompt for a file name:



Enter the file name and click on *OK*.

2.5. CALCULATIONS

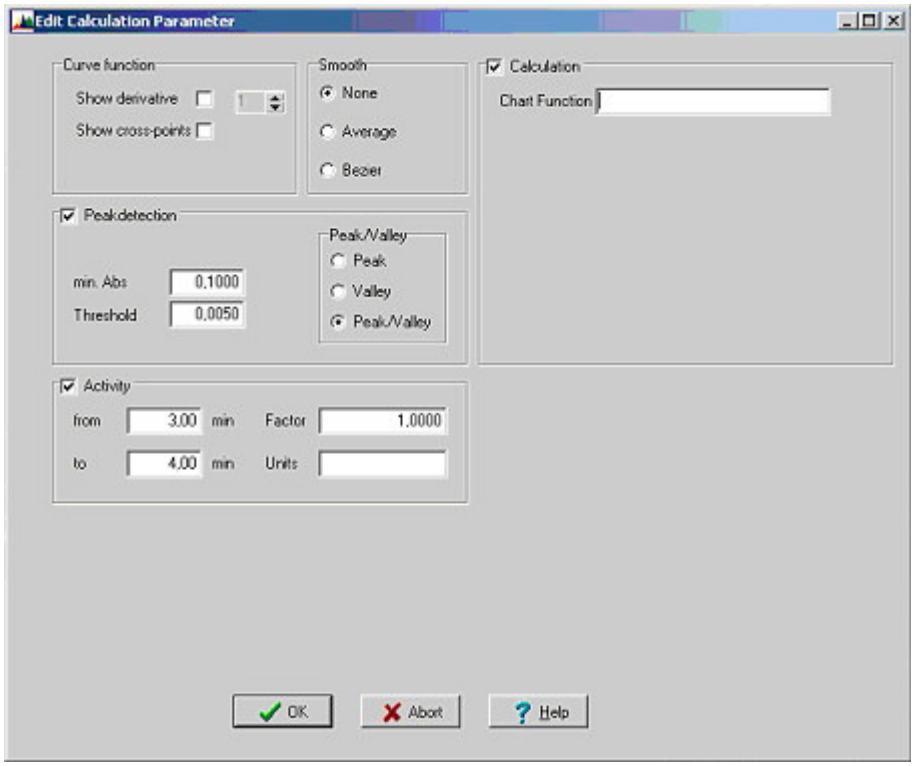
The UVS software contains various calculation possibilities depending on the selected measuring mode.. These calculations are accessible using the *Calculator* icon.

2.5.1. Curve Functions

Calculations based on charts can be executed in one of two ways:

- Post-run by clicking on the *Report* tab in the report section and then the calculator icon in order to obtain the calculation dialogue.
- Definition of the required calculations as a part of the method in which case they can be executed automatically at the end of the run.

Click on the calculator icon in either the *Method* or *Report* screen in order to obtain the calculation dialogue:



The functions available for manipulation of curve data are the following:

- Derivatives up to 4th derivative
- Cross-points
- Smoothing
- Mathematical calculations on a complete curve
- Peak detection
- Activity

2.5.1.1. Derivative

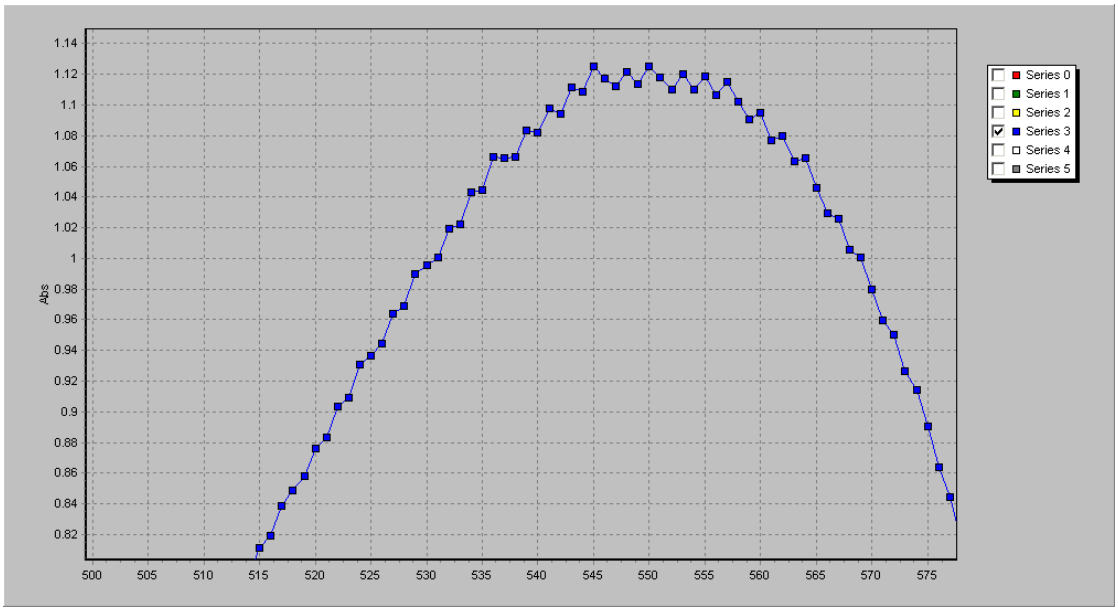
The software allows direct calculation of derivative orders 1 to 4 for *Wavelength Scan* and *Time Drive* data. A separate optimised calculation algorithm is used for each order therefore the quality of the result will be much improved if you calculate, for example, a fourth derivative directly from a loaded zero order curve.

To display a derivative click on the “Show derivative” checkbox, which will open the spinbox for selection of the required order.

Set the required derivative order in the spinbox and click on OK. The curve display will automatically change to show the new derivative curve.

2.5.1.2. Show cross-points

Selecting the *Show* cross-points parameter will display each data point collected on the curve as shown in the zoomed example below:



2.5.1.3. Smoothing

A filter can be introduced in the data acquisition in order to reduce noise. Smoothing can be selected with as an averaging or a Bezier function.

High smoothing will reduce noise, however high smoothing will also reduce the amplitude of the peaks obtained and can also result in distortion of peak shape.

Average This is a rolling average function based on 3 calculated points. Only Y values are calculated.

$$P(x) = [x_{(n-1)}+x_{(n)}+x_{(n+1)}] / 3$$

Bezier A Bezier curve is an approximation to a curve which would pass through all the control points. The method used here for defining such a curve approximation is called the Bezier-Bernstein approximation.

Savitzky-Golay
The fundamental idea is to fit a different polynomial to the data surrounding each data point. The smoothed points are computed by replacing each data point with the value of its fitted polynomial.

For the smoothing functions “Average” and “Savitzky-Golay” three smoothing degrees can be selected:

Low – Medium – High

2.5.1.4. Calculation

The calculation function allows definition of mathematical functions which can be used to modify the curve data. “S” is used to denote the sample itself and calculations are defined simply using “S” and the appropriate factor (F) and signs:

Addition:	Enter	F+S
Subtraction:	Enter	S-F
Multiplication:	Enter	F*S
Division:	Enter	S/F

For example it is also possible to subtract an offset from each point in the curve and then double the signal level and this would be programmed as follows:

Click on the *Calculation* checkbox and then enter the required formula, in this example the formula would simply be 2*(S-0.2).

Caution *Please note that spaces are not permitted in the formula.*

2.5.1.5. Peak Detection

This calculation mode can be used with the system methods: *Wavelength Scan*, *Time Drive* and *Auto Rate Assay*.

Peak detection can be linked to a method and carried out during or after measurement. To activate peak detection select **“Peak detection”** in the calculation parameter editor window.

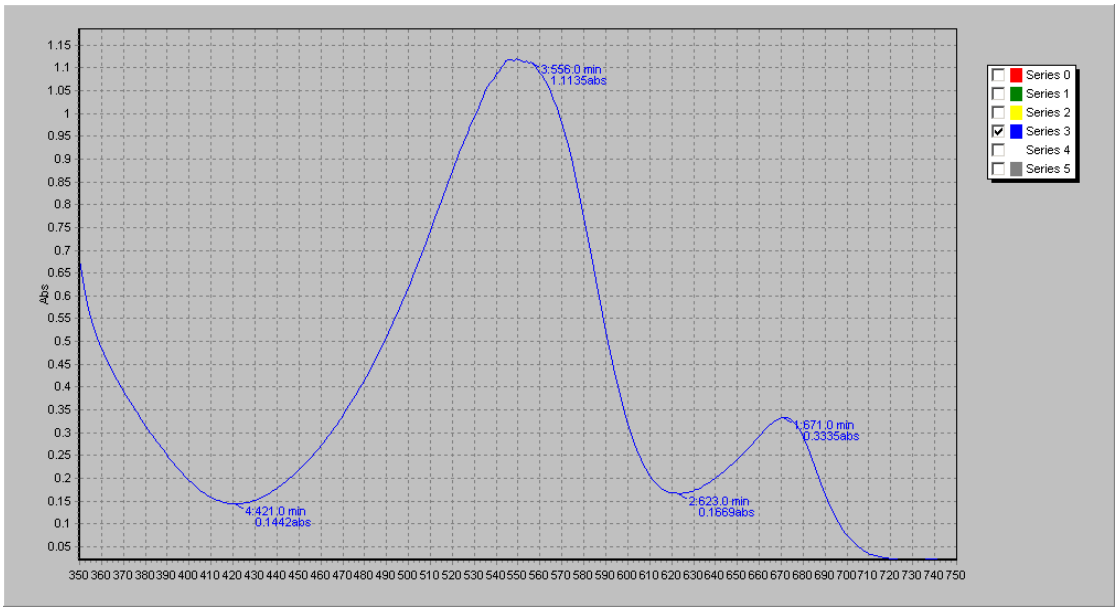
A peak is detected when the slope of the curve changes from positive to negative, a valley is detected when the slope changes from negative to positive.

After selecting **“Peak detection”** it is possible to set the following parameters:

Min. Abs The Min. Abs. parameter defines the absolute minimum value for a peak or valley to be detected, any peak or value with an absorbance value lower than the defined value will be ignored.

Threshold The threshold is the difference in height on the Y-axis between two peaks or valleys. If the difference between valley and peak is lower than the set threshold then the peaks/valleys will not be detected.

Peak / Valley The selection defines whether the calculation is to be made for peaks only, valleys only or both peaks and valleys.



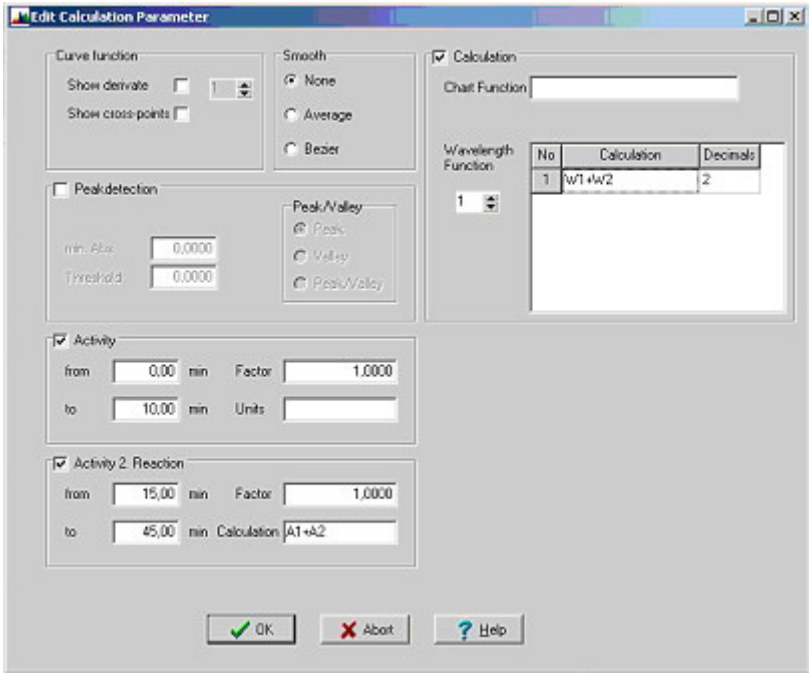
If peak detection has been selected the results can be seen both in the peak detection table and directly on the curve itself:

2.5.2. Activity

This calculation mode can be used in the system methods *Time Drive* and *Auto Rate Assay*. An activity of the second reaction can be used exclusively in the system method *Auto Rate Assay*. It is used to calculate the activity of reactions. Calculation of the activity is made using a linear regression model.

The calculation can be embedded in the method such that it is performed automatically at run end or it can be executed manually after acquisition.

Selection of the parameters for the *Activity* calculation is made, as above, by clicking on the *Calculator* icon in either the *Method* or *Report* screens. Click on the *Calculator* icon to obtain the appropriate dialogue box and then click on the *Activity* checkbox.



It is possible to define the section of the curve over which the calculation is to be made, a factor and the units for the *Activity* value:

It is now possible to set directly the following parameters:

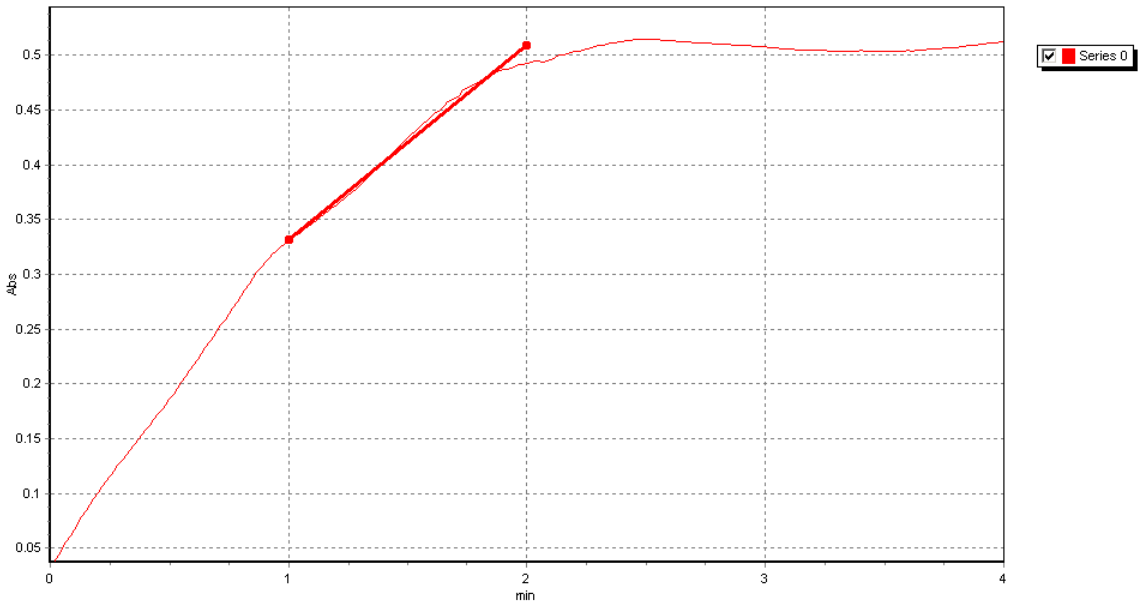
From Defines the lower starting point on the curve time-scale for the range of the *Activity* calculation.

to Defines the upper starting point on the curve time-scale for the range of the *Activity* calculation.

Factor Activity is calculated by multiplying the slope of the regression line (Absorbance change per minute) by the factor (**F**).

Units Defines the units to used for reports etc., e.g. Abs/min., µmol/min

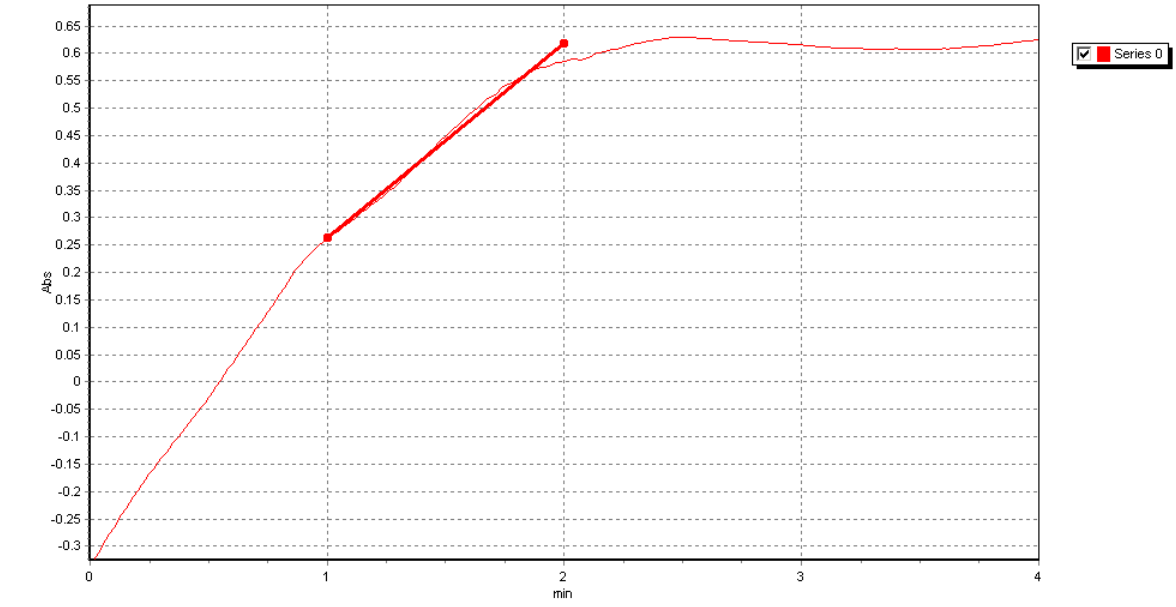
Using the above example the curve obtained would appear so:



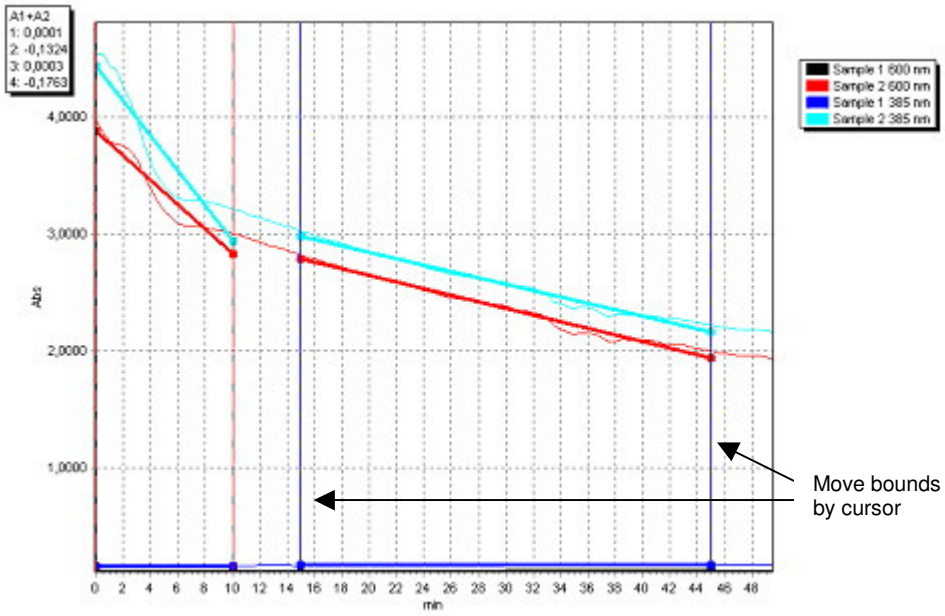
All curve calculation functions described above can also be used to modify curves used for the activity calculations.

For example it would be possible to subtract a pre-determined *Blank* value from the curve and then multiply it by a different factor, in this example the formula could be **2*(S-0.2).**

This would give the following result:



An example for defining two activities would appear so:



The bounds for activity calculation may be moved by the cursor with real-time calculation. Activities can be calculated with a mathematical function.

2.5.2.1. Activity Results

The results of the activity calculation over the requested time period can be viewed by clicking on the *Activity* tab in the *Report* screen. This displays the actual activity value for the sample plus the calculated regression line and also the correlation coefficient.

In addition the *Table* tab will show the actual activity at each point on the curve with respect to the last value. For the point n on the curve at a time t_n and an absorbance value of Abs_n the activity is calculated as

$$\mathbf{Activity = (Abs_n - Abs_{(n-1)}) / (t_n - t_{(n-1)})}$$

2.5.3. Concentration Factor

This is the most simple calculation method for concentration and is used in *Fixed Wavelength*. The concentration factor must be determined in advance if this calculation is to be used. The system uses this factor and performs the following calculation:

Concentration = Measured Absorbance value x Factor

The factor is entered as a parameter in the Acquisition screen. Click on the parameter tab to enter the screen and then enter the required value for the factor.

In this case no calibration file is required and the factor used is recorded in the report.

2.5.4. Wavelength Program functions

The *Wavelength Program* calculation functions apply only to this mode of operation and are described in the *Wavelength Program* section of this document. One more parameter appears in the calculation column.

2.5.5. Linear Calibration

The *Calibration* mode is used to create standard calibration files for the *Fixed Wavelength* mode. The *Calibration* uses a standard *Fixed Wavelength* method which must be created before running *Calibration* mode.

Method creation is possible in both the *Fixed Wavelength* and *Calibration* method screens. A method can be used to create as many calibration files as needed, the method and revision used is always linked to the calibration and is traceable.

The *Calibration* procedure is best explained using an example. In this example we will use a blank and two standards. The calibration can also be made using the cell changer.

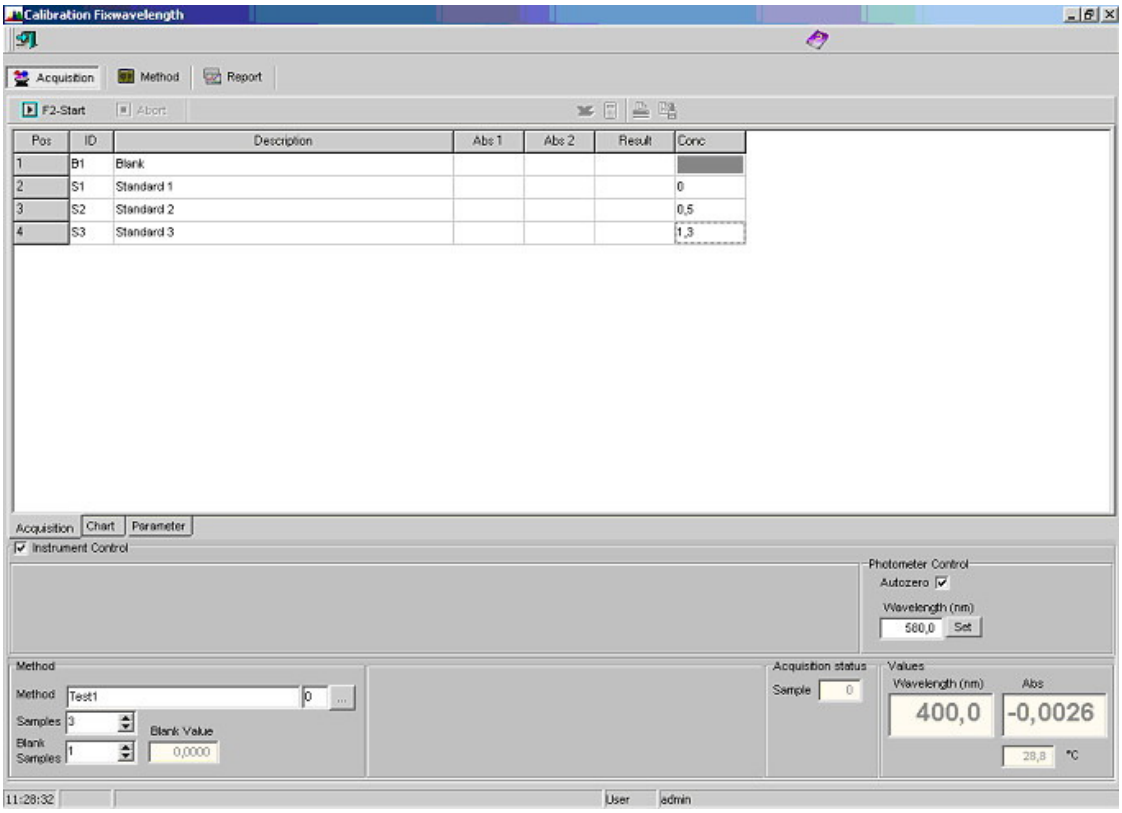
2.5.5.1. Creating a Calibration File

Select the *Calibration* mode by clicking on the *Calibration* icon in the main screen and insert the blank and the two standards in the cell changer at positions 1, 2 and 3.

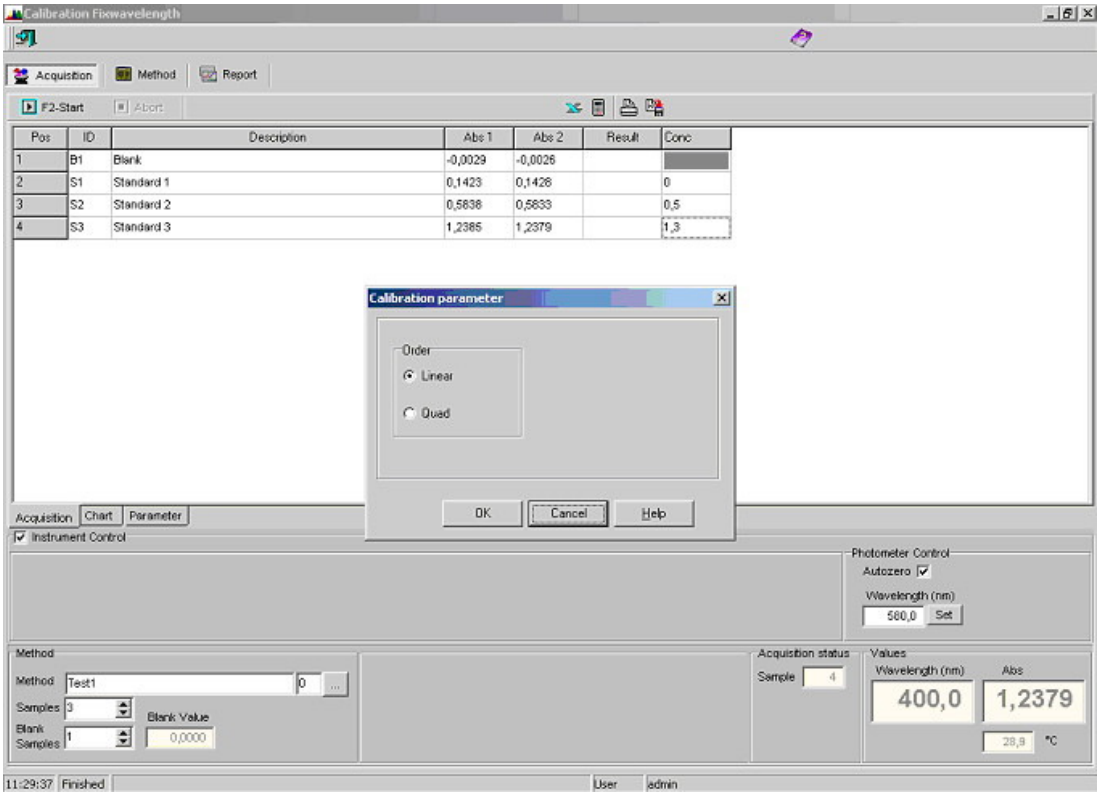
Enter the number of samples (3), the required method, a description of each sample and the concentration in the main Acquisition screen.

Clicking on the *Parameter* tab will allow entry of the units to be used for the result and also definition of an additional multiplier factor which will be used to multiply the value obtained to give the result..

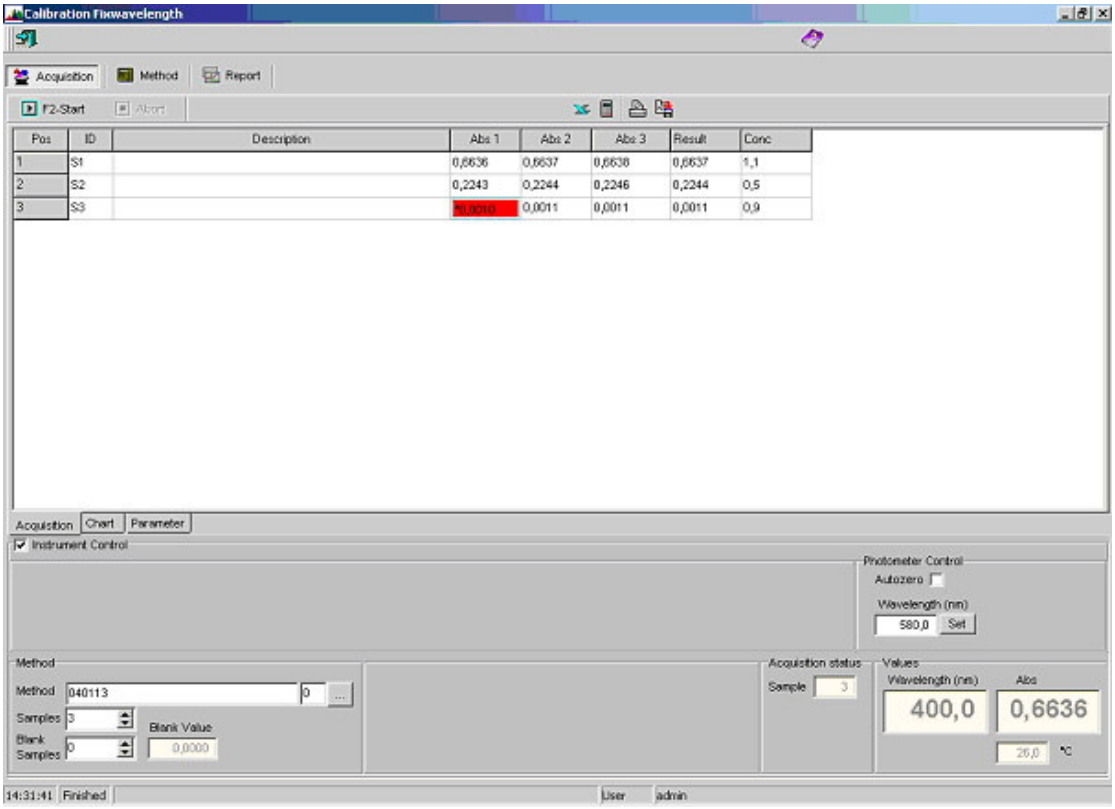
The final screen will look like this:



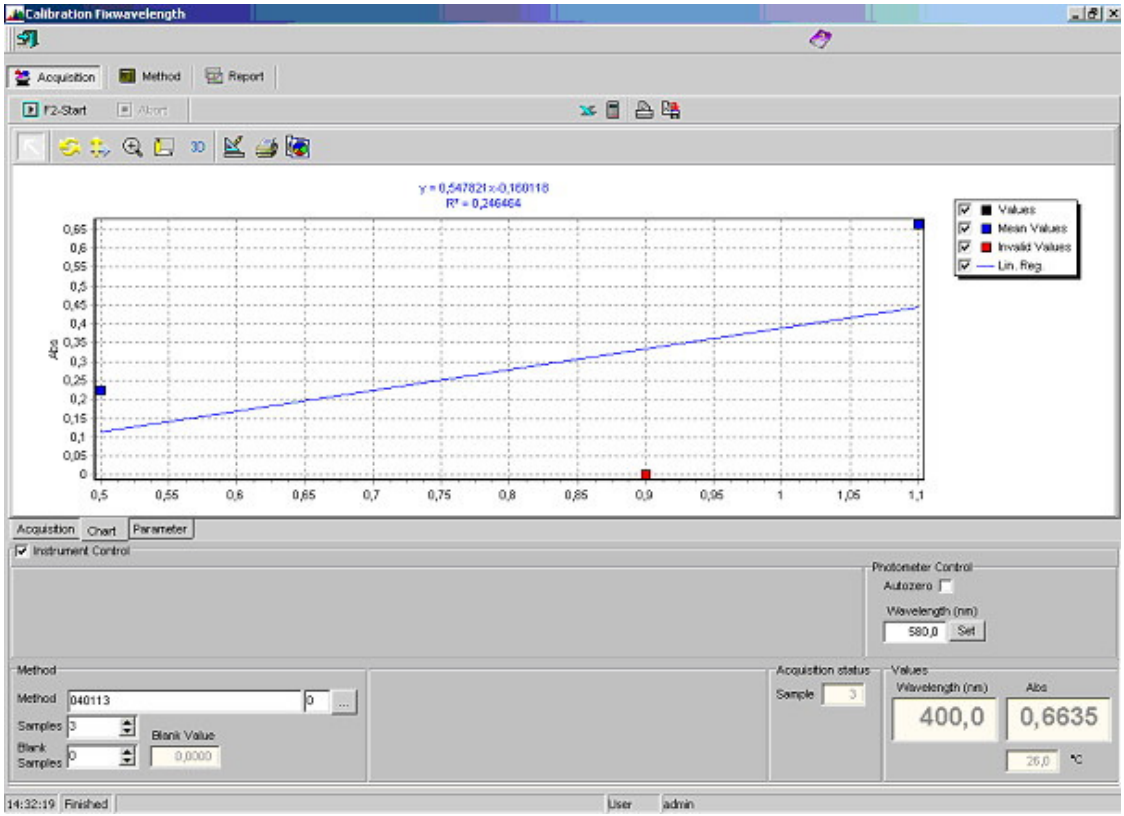
Click on *Start* to start the acquisition. Once completed the system will automatically prompt for the type of calibration required. Two possibilities are available using either a linear or quadratic regression:



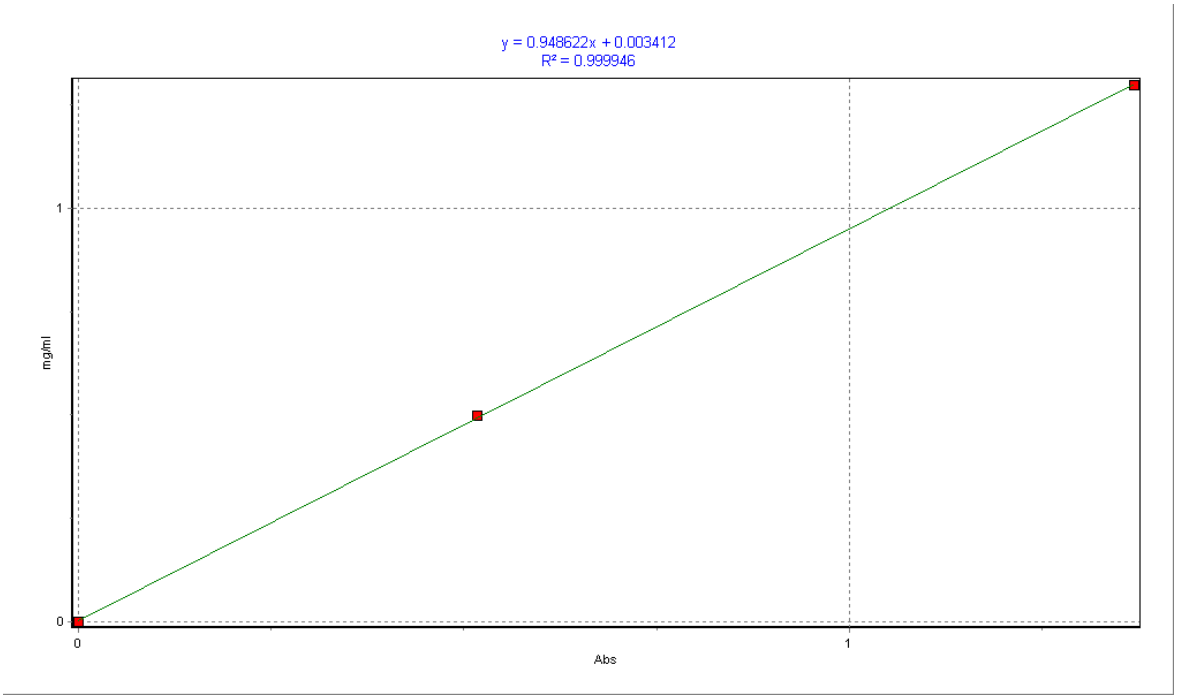
The Calibration parameter dialogue box can be recalled at any time by clicking on the calculation icon. Click the *Linear* checkbox and then save the calibration under the name required.



Values may be invalidated by double-clicking them. Invalidated values and their respective measure points in the *Chart* are marked red.



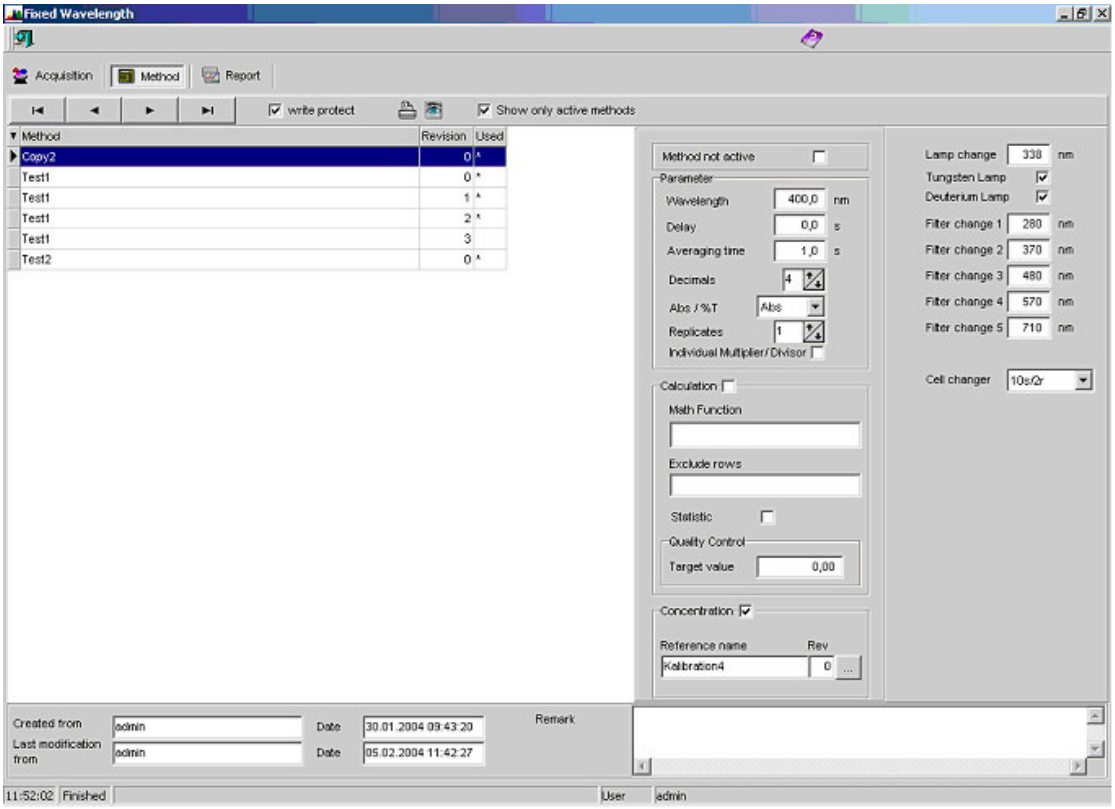
The data for a calibration can be viewed at any time by selecting the required report in the *Report* screen. Click on the Chart icon and the calibration curve will be displayed together with the regression values:



2.5.5.2. Using a Calibration Curve

The calibration curve can now be used to measure a series of unknown samples:

Exit the *Calibration* mode and select *Fixed Wavelength* and then select the *Method* screen. Here you should click the *Active* checkbox in the *Concentration* and then select the required *Calibration* as *Reference data*. Save this method and the screen should look like this:

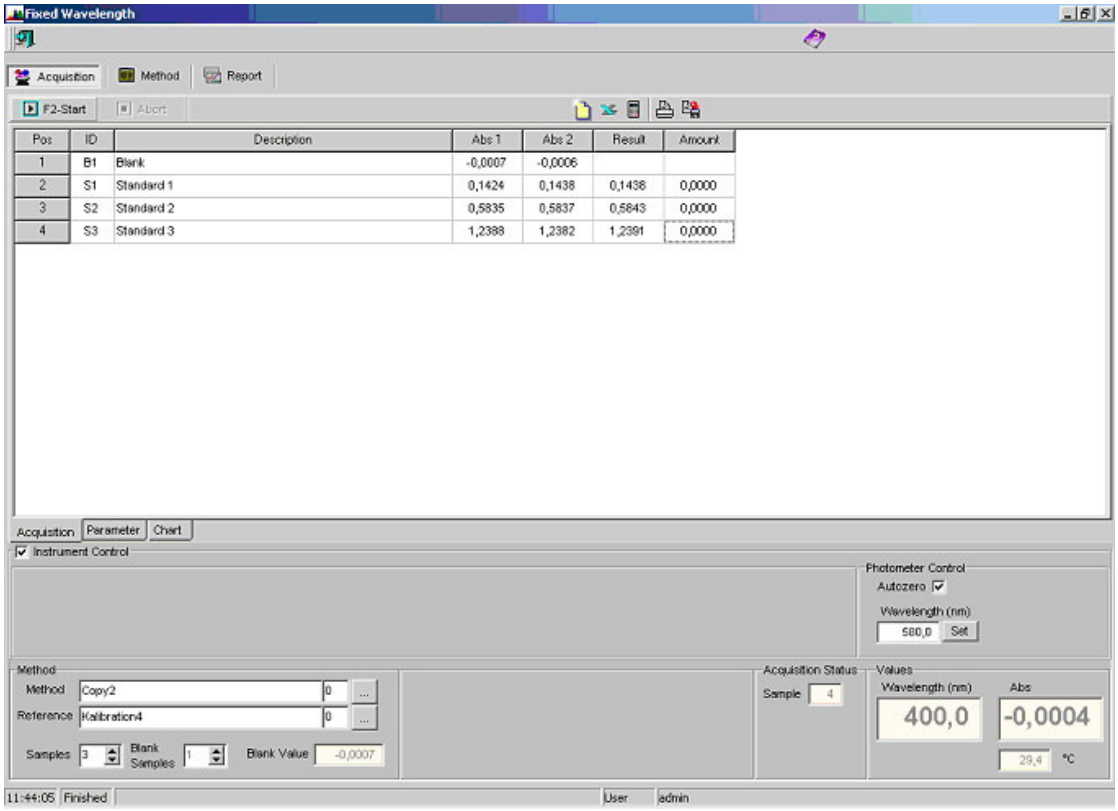


Select the *Acquisition* screen, insert the samples in the cell changer and set the number of samples to the appropriate value.

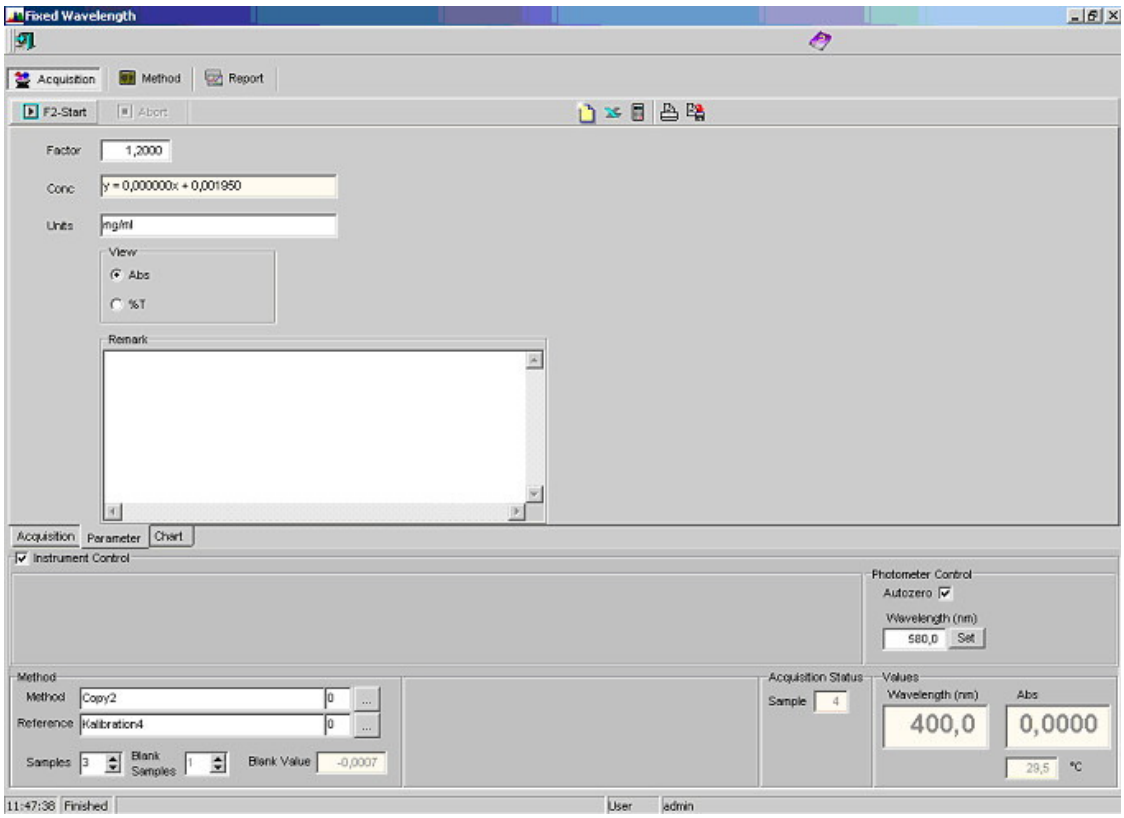
Check whether an *Autozero* is required before starting the measurement If so, click the *Autozero* checkbox in the *Acquisition* screen

Caution *Before executing the Autozero ensure that the cell changer (if used) is actually in the correct position. The Autozero will be executed at the current position which may not be position 1. Measurements with the cell changer always start from position 1.*

Press *Start*, after measurement the *Acquisition* and *Parameter* screens obtained are shown below. The main screen contains the measured absorbance values, the result and the calculated concentration values:



The *Parameter* screen contains the value used for the *Factor* used to obtain the result, the formula used to calculate the actual concentration and also the units (e.g.: µg/ml, mg/ml, etc.) may be entered:



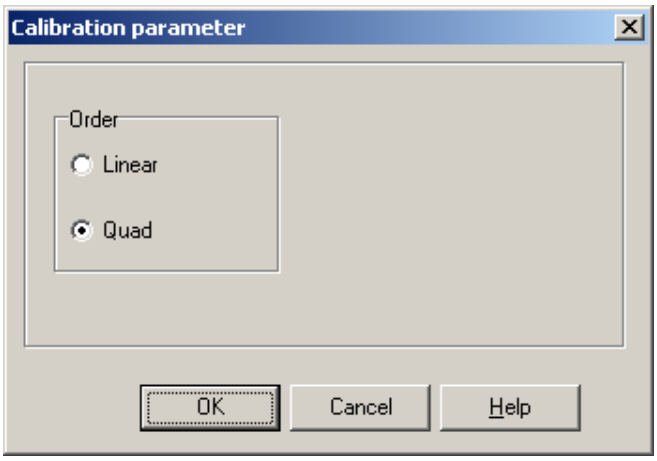
2.5.6. Quadratic Calibration

(Calculation of concentration by quadratic regression using standards)

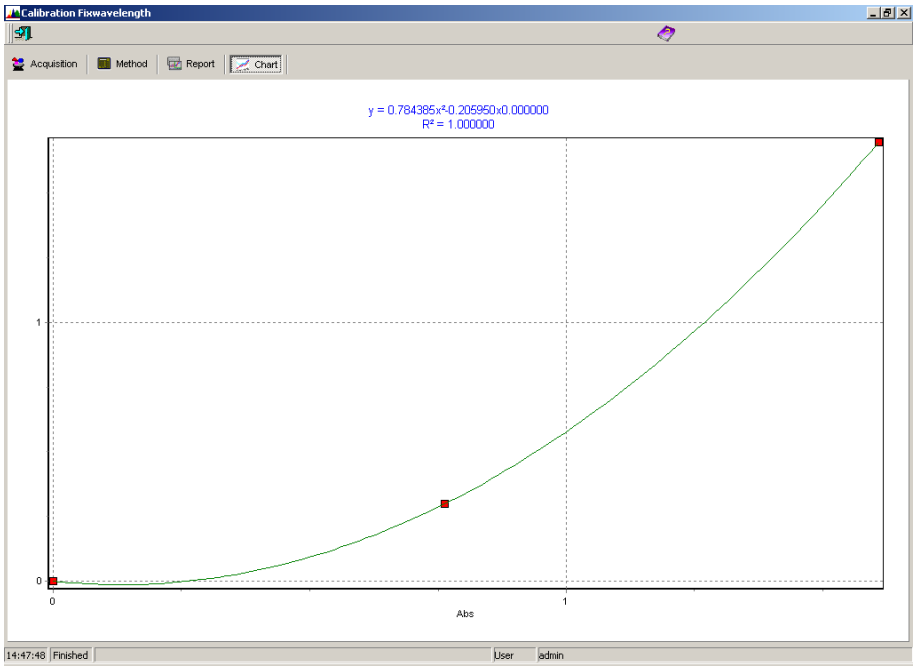
The practical use of this calculation mode is almost identical to linear interpolation (see above). One additional parameter is used with the following formula:

$$Y = Ax^2 + Bx + C$$

The process of obtaining the calibration data is identical for both the *Linear* and *Quadratic* calibration methods until selection of the calibration order is made.
Select the *Quad* function in the *Calibration* parameter dialogue:



The calibration curve will now look like this:



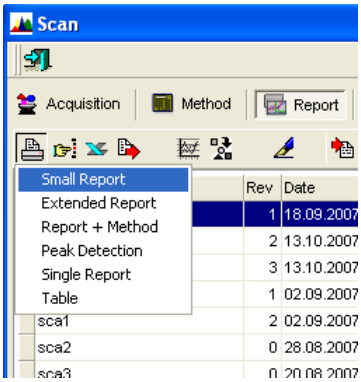
2.6. REPORTING

This section deals only with the possibilities for formatting and printing reports in the UVS software. The main focus is on the treatment of curves since all table format printouts are pre-defined.

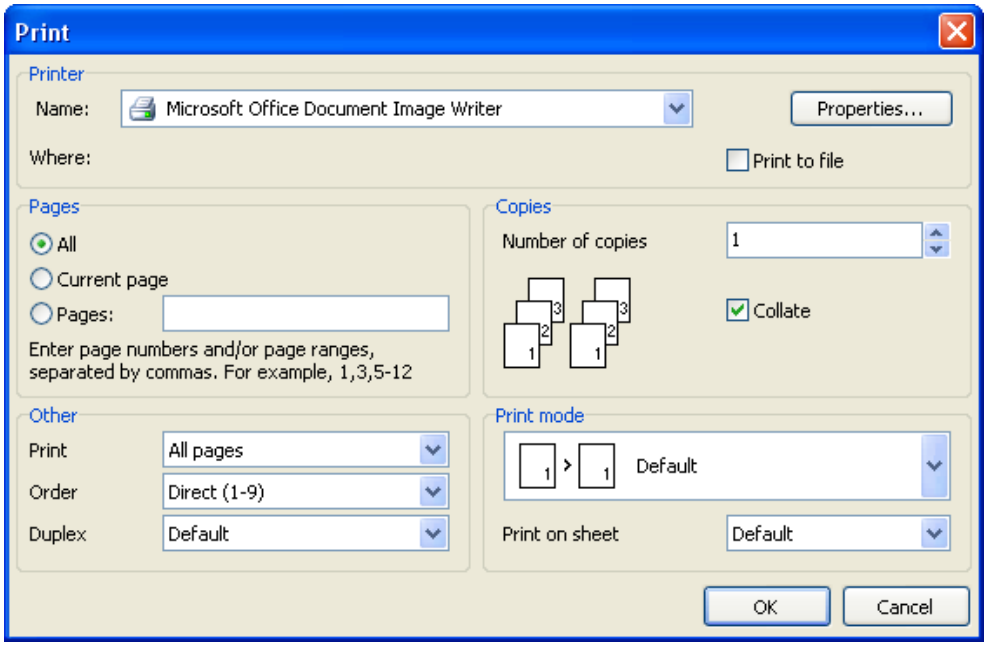
2.6.1. Printing

The UVS software offers several possibilities for printing and formatting the various reports and data available from the system. Individual print-outs are possible for method parameters, individual results e.g. peak detection, complete reports and curve data. Each window contains its own *Printer* icon which gives a preview of the print-out.

Within the preview page the user also has the possibility to save reports under user-defined names and these reports can be viewed using the viewer of the UVS software. Click on the *Print* icon in the report screens and you will be prompted for selection of the report type required:

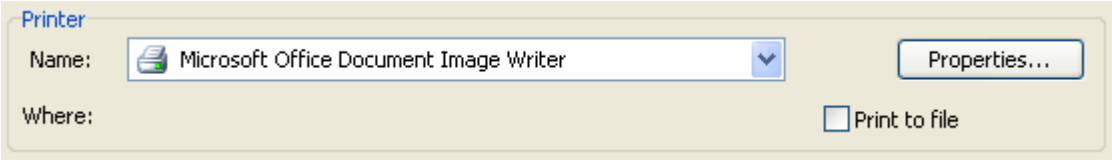


The window appears – it is printing dialogue.

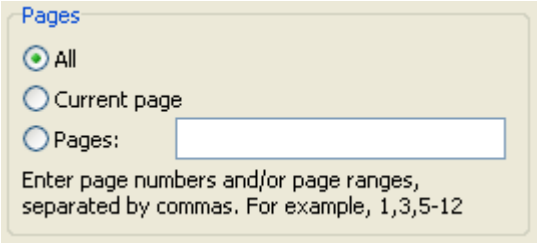


Let's look at options available in this dialogue.

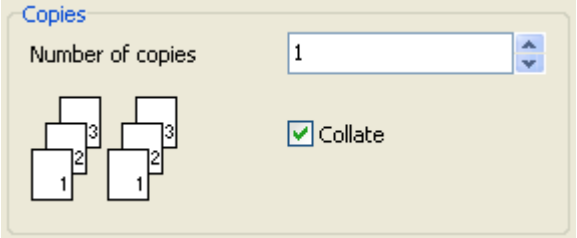
The "Printer" group: you can select a printer via which you want to print a report; set printer properties, for example, printing quality; and choose print to file.



The "Pages" group: you can select which pages to print (all, current, selected range).

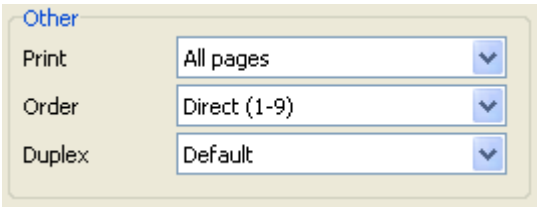


The "Copies" group: you can set how many copies to print. If Collate flag is set and you choose to print several copies, at first one report copy is printed, then – the next etc. If flag is disabled, several copies of the first page are printed, then – several copies of the second one etc.

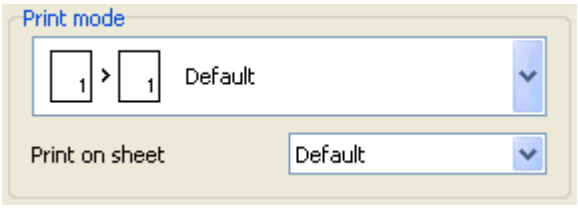


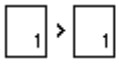
The "Other" group:

- Print - you can select which pages to print. Variants: All pages, Even pages, Odd pages.
- Order - print pages in direct or reverse order (from last to first page).
- Duplex - handle duplex by default (report settings are used) or choose one of duplex options: vertical, horizontal, simplex.

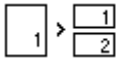


The "Print mode" group: you can select one of the printing modes.

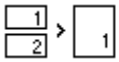




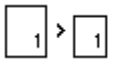
- Default mode. The printer prints on the sheet defined in a report. One preview page is printed on one sheet.



- Split big pages. This mode is useful if you need to print A3 report on A4 sheet. One preview page is printed on several sheets. If you choose this mode, you have to choose the sheet size ("Print on sheet") as well.



- Join small pages. This mode is useful if you want to print A4 report on A3 sheet. Two or more preview pages are printed on one sheet. If you choose this mode, you have to choose the sheet size ("Print on sheet") as well.



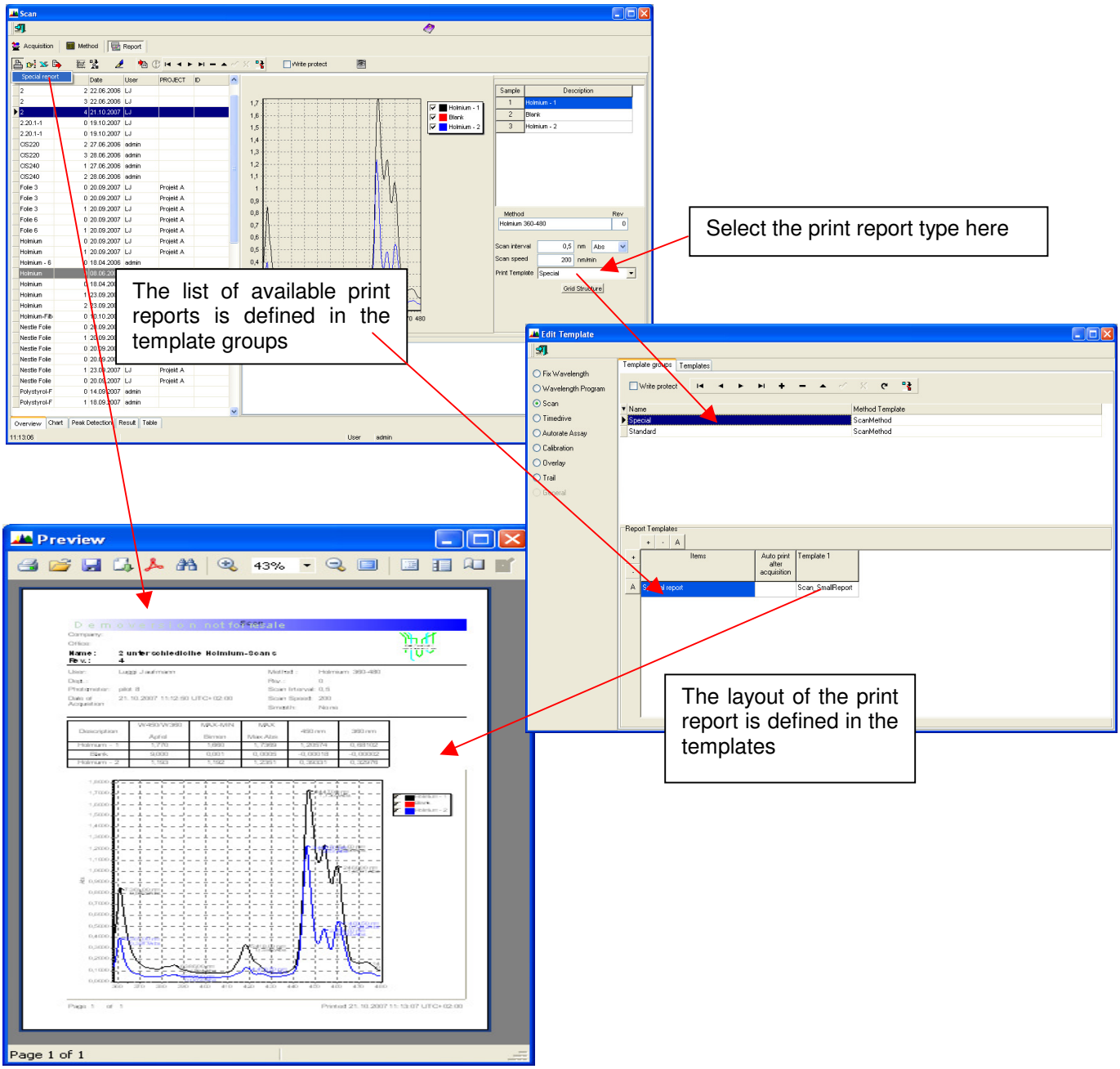
- Scale mode. Report is printed on specified sheet. All report output is scaled. One preview page is printed on one sheet. If you choose this mode, you have to choose the sheet size ("Print on sheet") as well.

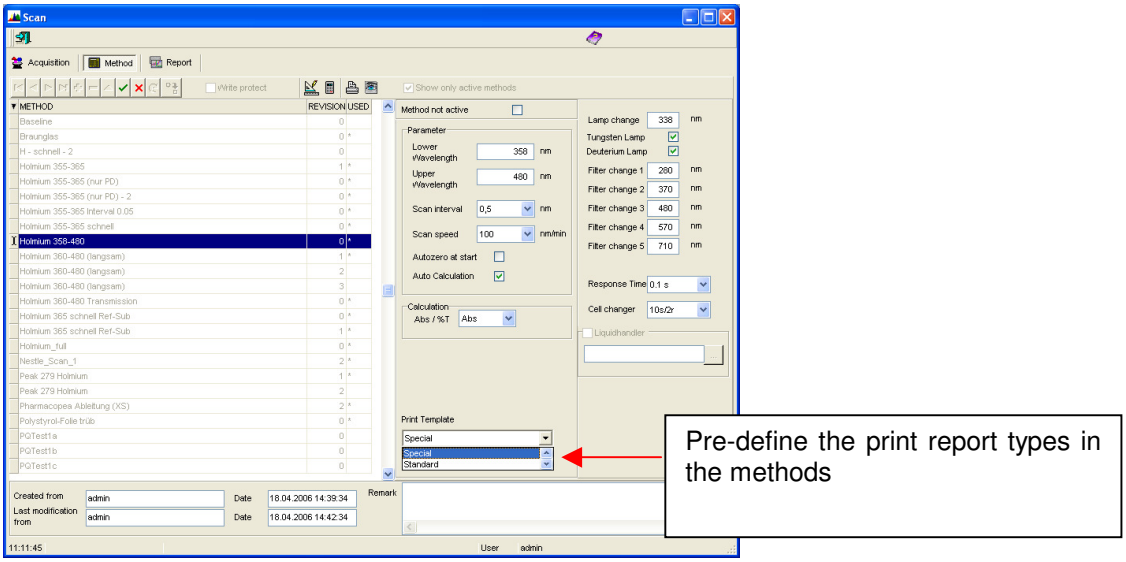
After clicking on OK report printing begins. If the “Print to file” flag is selected, file name is called. And report is saved to this file (file with *.prn extension. It contains a copy of information sent to printer).

2.7. REPORT MANAGER

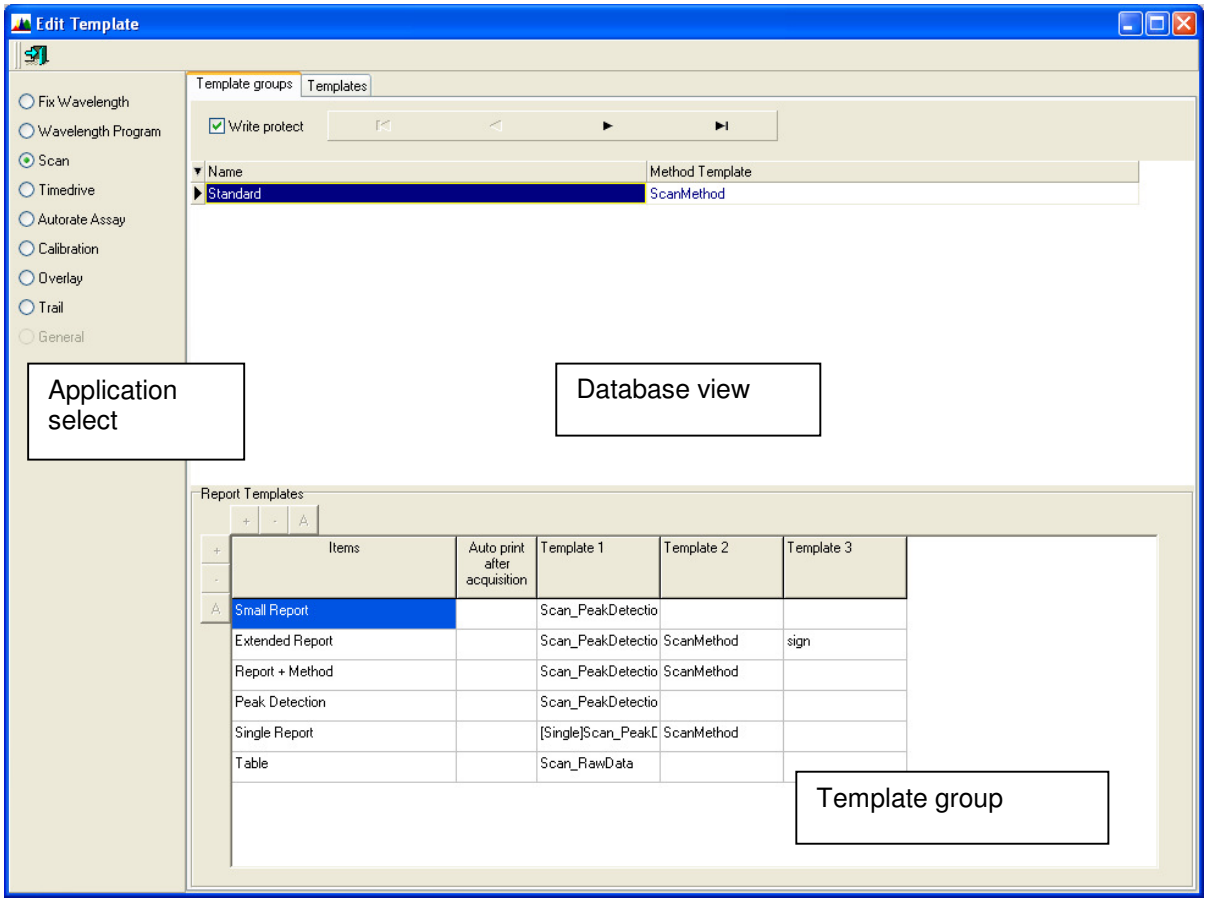
The report manager is supplied with an embedded designer, which can be called in design-time by double-clicking on templates. The designer provides the user with all the tools for designing a report's appearance. It contains several toolbars, which can be docked wherever you want.

The report manager takes the contents of the templates and join it with data from the application.


Select the print report type here
The list of available print reports is defined in the template groups
The layout of the print report is defined in the templates
Page 1 of 1



2.7.1. Templates

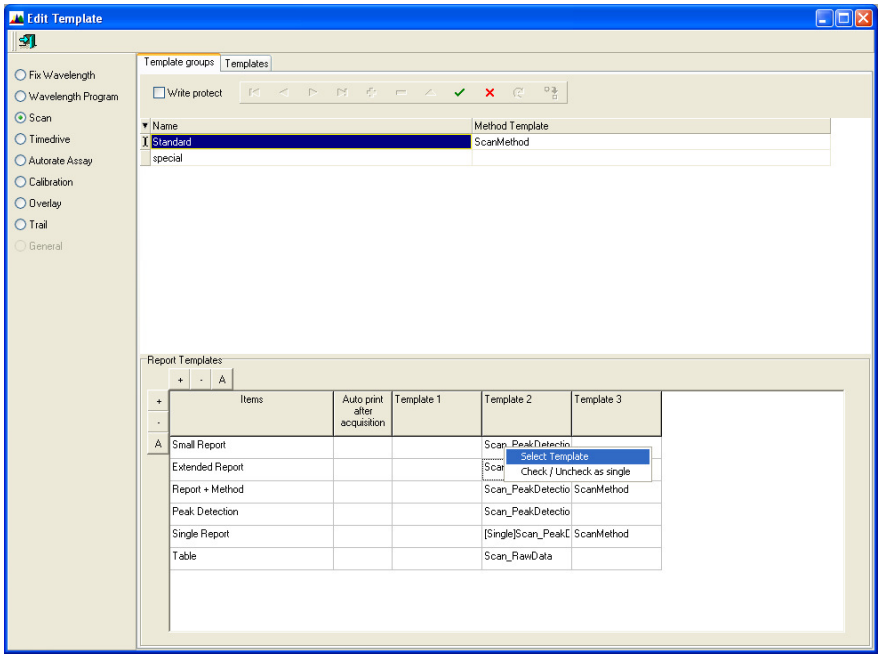


Application select: You can choose between different applications, like Fix Wavelength,Wavelength program, Scan, ...

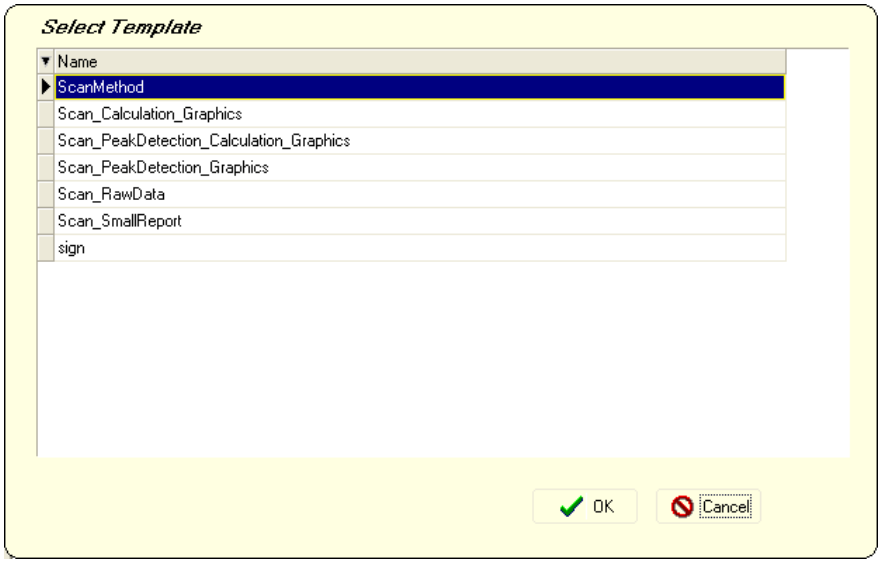
Database view: Here you can select and add template groups.
To add a template group, please uncheck „Write protect“ on the top and push the + button on the task bar.
To delete a template group push the – button on the task bar.

Template group: For inserting a template group at the selected cell push the right + button under „Report Templates“.

To delete a template group click on the right – button under „Report Templates“



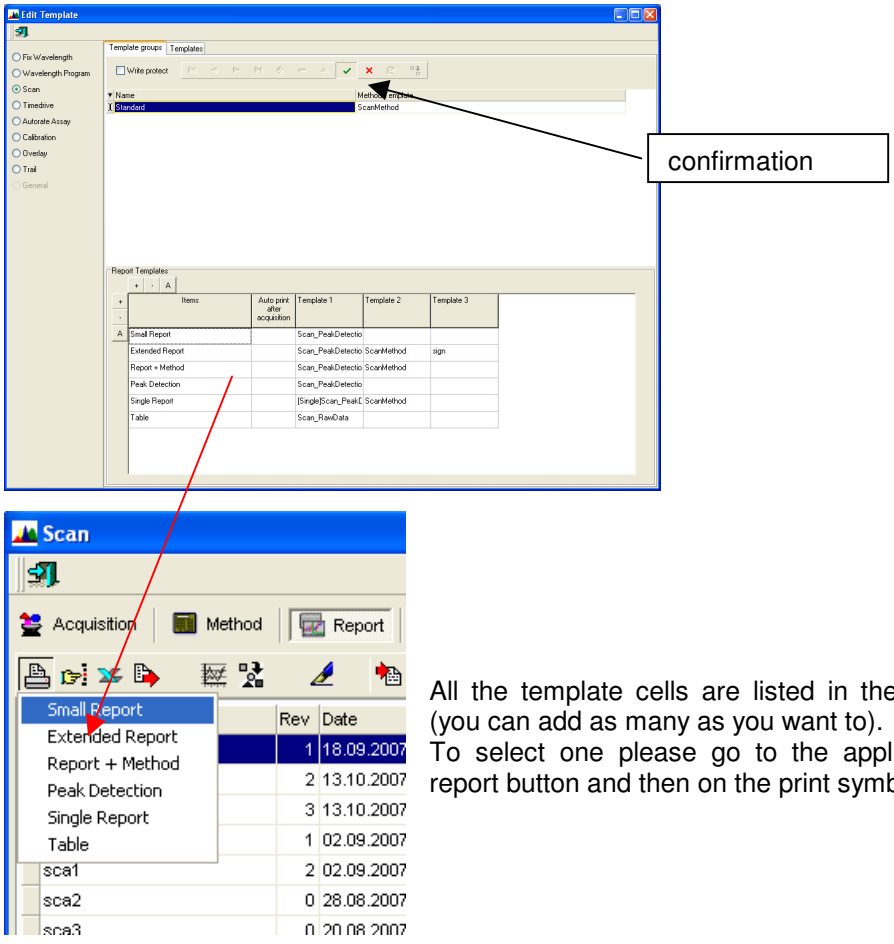
To add a new template, please first select your template cell and now click the right mouse button to show the selection possibilities. Choose „Select Template“.



Confirm wtih OK Button

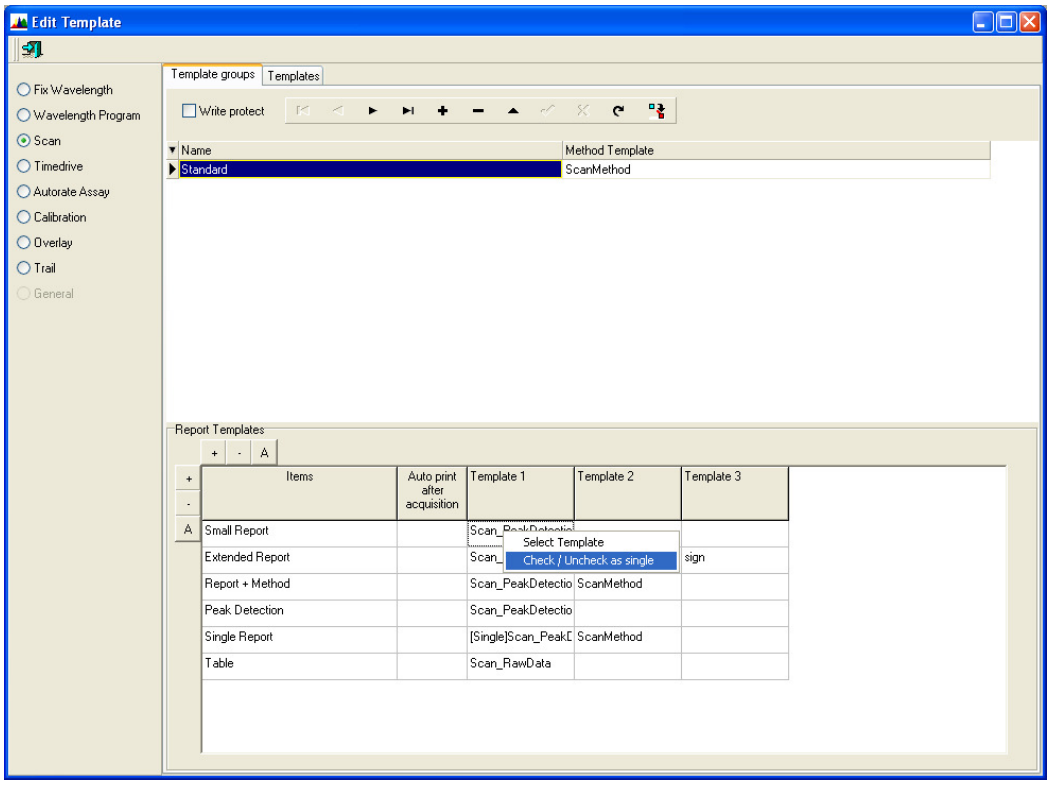
Now you can see the templates in one print report

Confirm all your actions with the green post-button on the top!



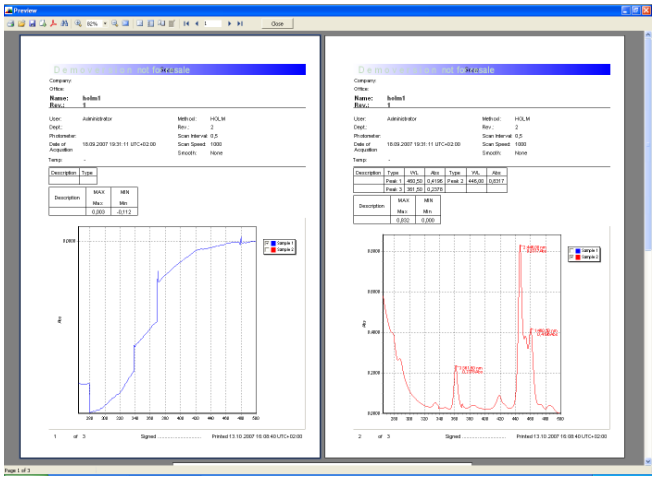
All the template cells are listed in the approbiated application (you can add as many as you want to).
To select one please go to the application and click on the report button and then on the print symbol.

2.7.1.1.1. How to print single curves in the applications Scan, Timedrive, Auto Rate Assay

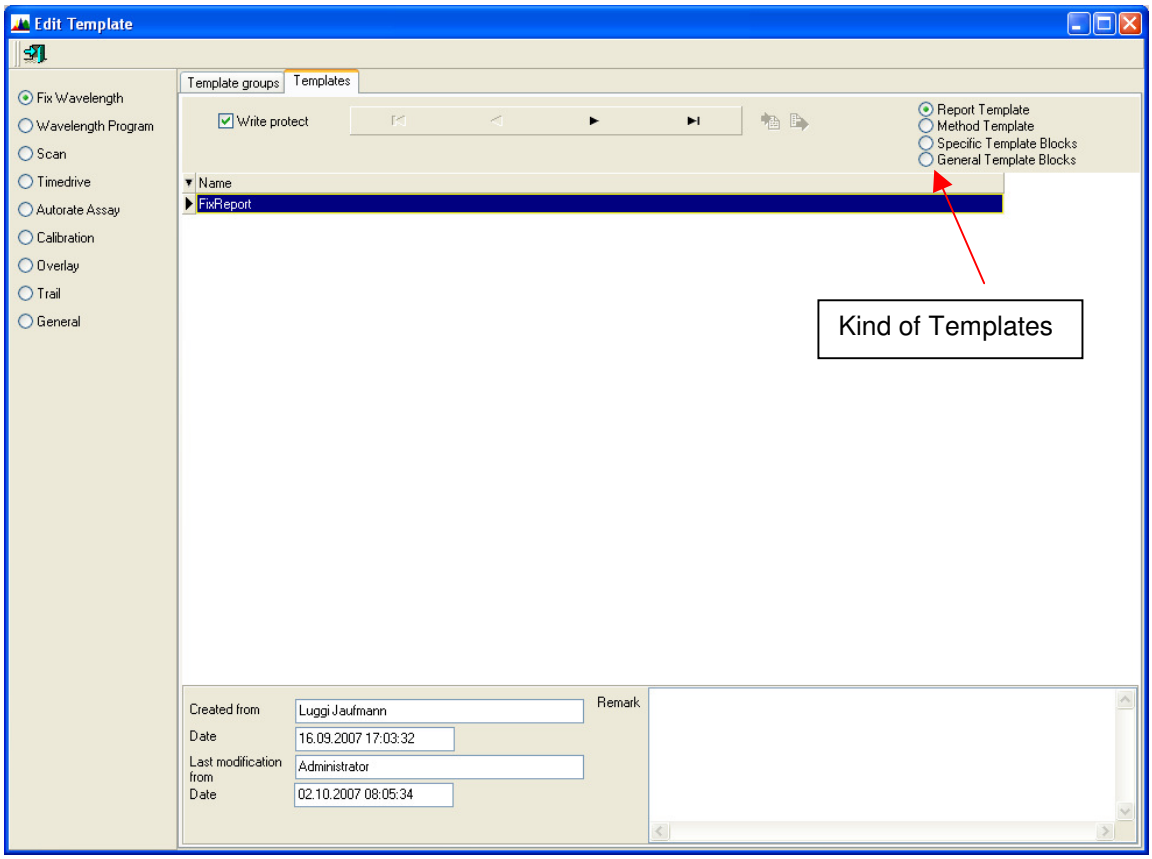


Define the apperance of 2 curves in the print report in one diagram or only a single curve in each diagram. To have only one curve in your diagramm click with the right mouse tab on your template and select „Check/Uncheck as single“. Now you have a new diagram for each curve in your print report (see on the bottom).

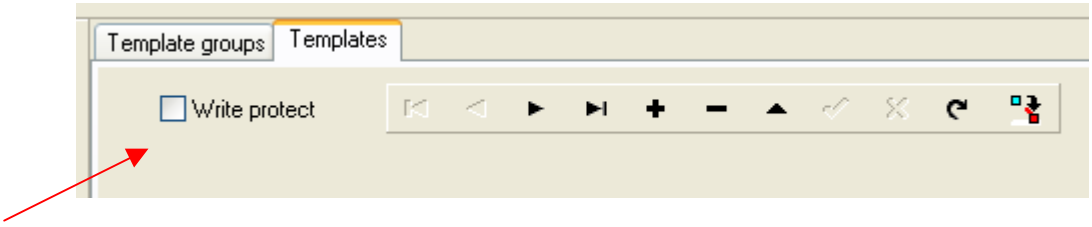
Single curves are only possible in the following applications:
Scan, Auto Rate Assay and Timedrive!



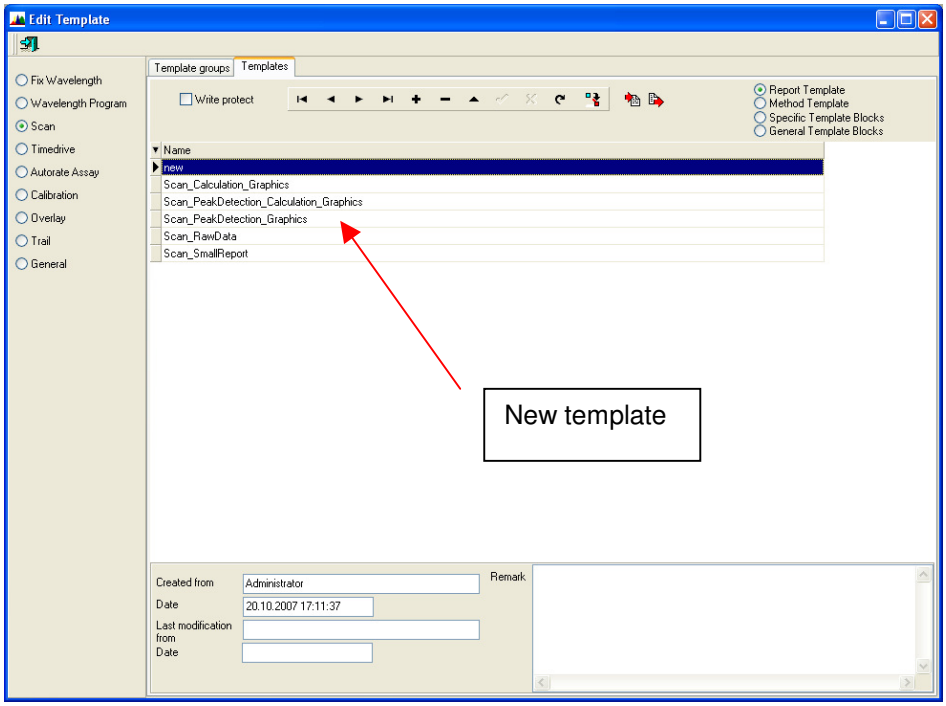
2.7.1.2. Create and select templates and template blocks



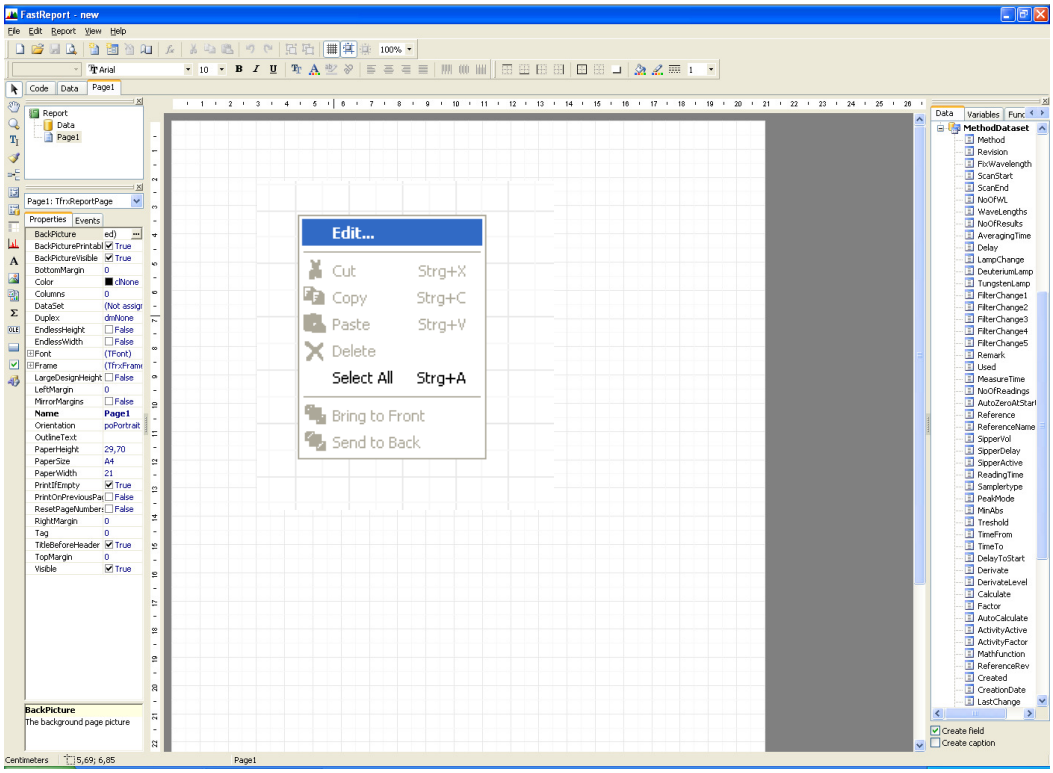
To edit and create new templates click on the tab „Templates“ and uncheck „Write protect“



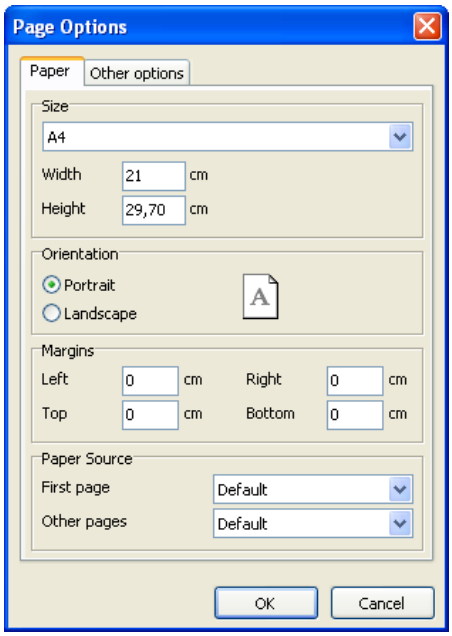
To create a new template click on the +Button on the task bar. Then you are asked to give the template e name.

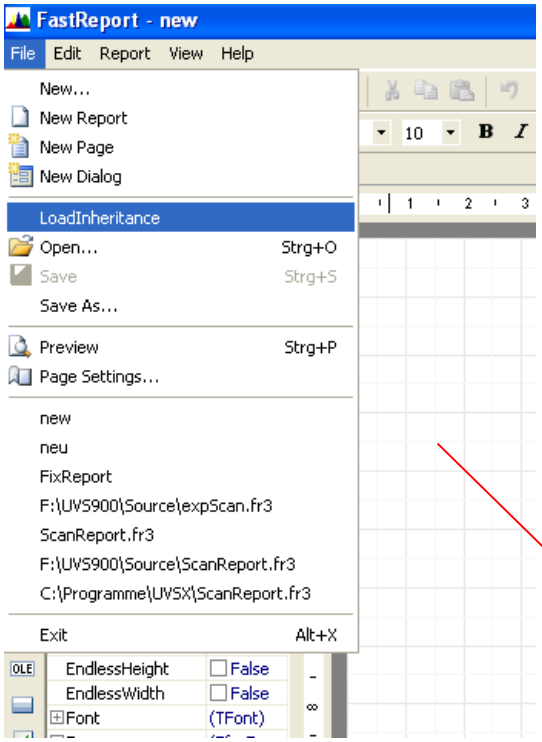


Choose the template you want to edit and double-click on it. A new window will be opened and shows the report designer.



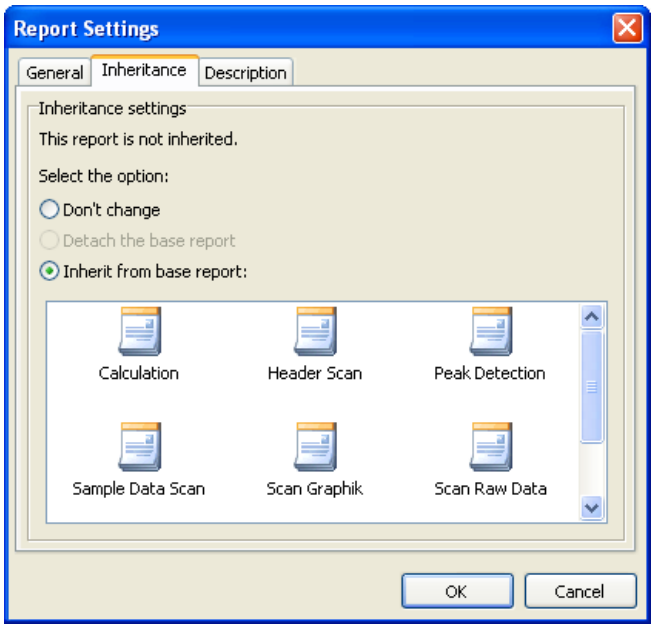
Edit the report options with clicking on the right mouse and select edit. Define now the page options like size, margins, orientation.



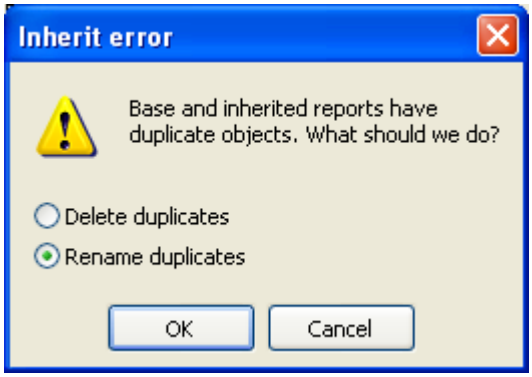


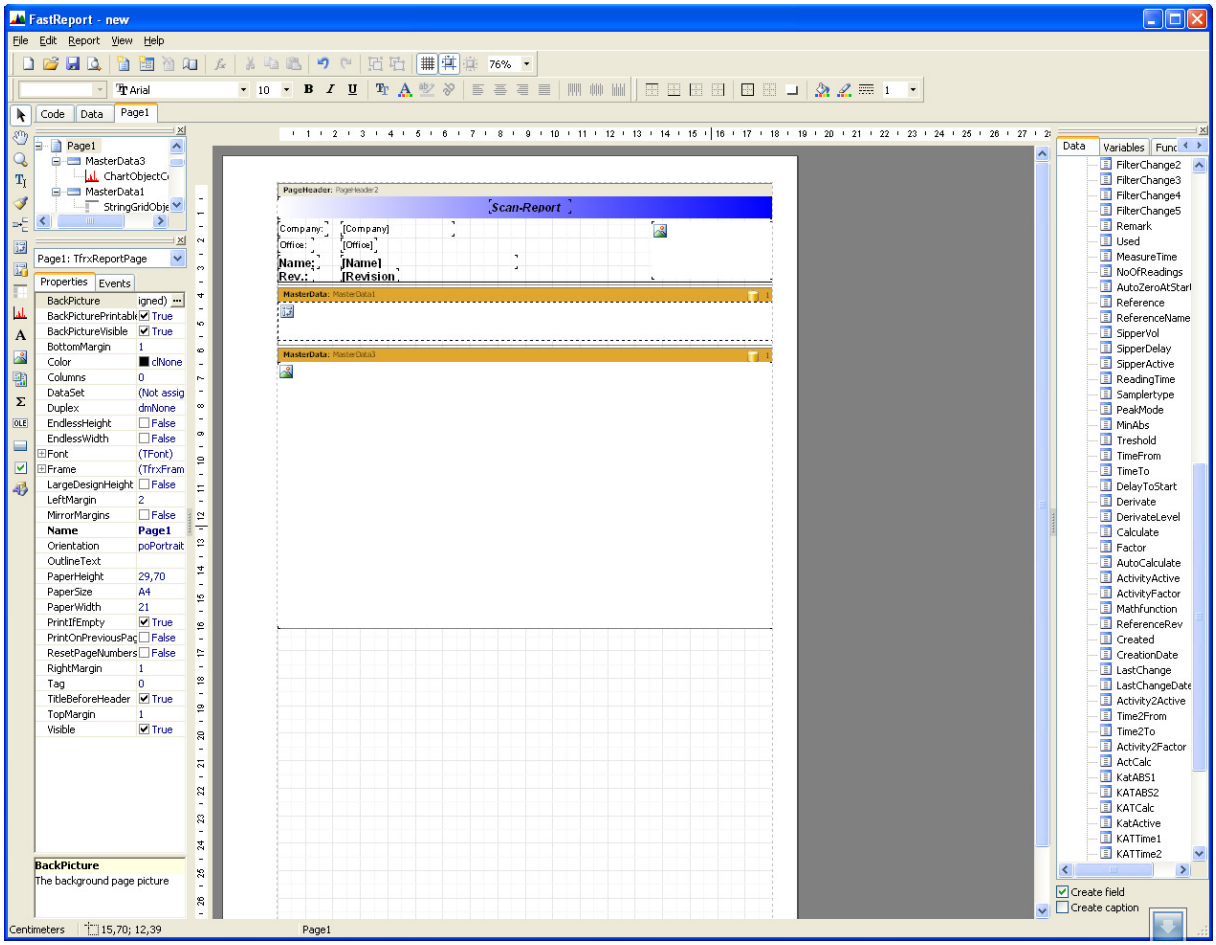
Click on „File“ and after then on „LoadInheritance“ to select the list of report blocks.

Here you can choose your report blocks.They appear in the report page in small blocks.



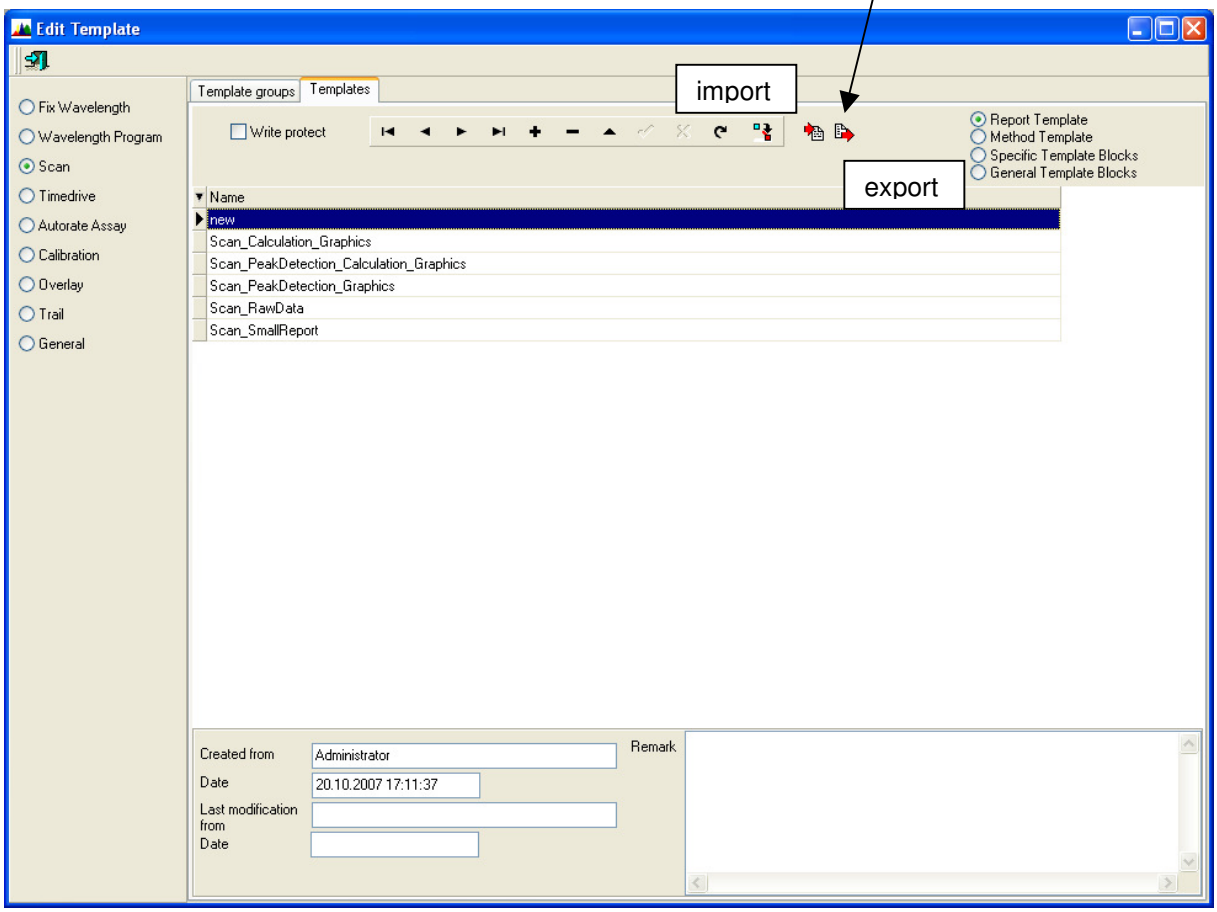
If there are objects with the same name are already in the template please select ‘Rename duplicates’ :





Add all the blocks onto the sheet you want to and click the save button for save and exit.

To import or export your templates please click on the following buttons in the task bar on the top.



2.7.1.3. *List of some predefined report templates*

Print extended document

This will give a complete report which contains also details of the complete method used and the signature box for electronic signature confirmation.

Print small document

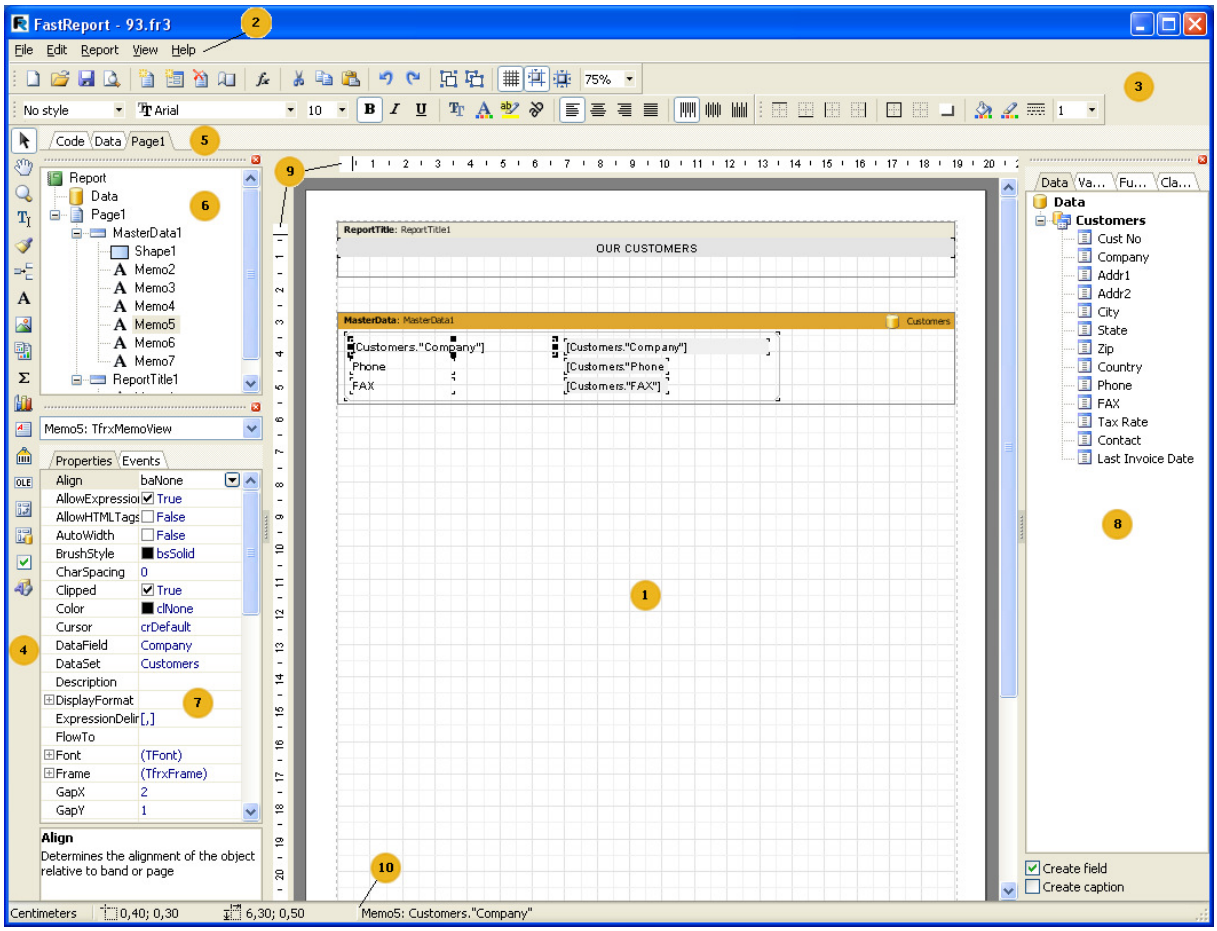
This is a report which contains only the basic results of a measurement and some other limited information regarding measuring conditions etc.

Print table

This report contains only the table of the measurement values and other data linked to the table.

2.8. Report design editor

The report component is supplied with an embedded designer, which can be called in design-time by double-clicking on the TfrxReport component. The designer provides the user with all the tools for designing a report's appearance, along with the ability of simultaneous previewing. Designer's interface meets up-to-date requirements. It contains several toolbars, which can be docked wherever you want.



In the picture, denoted with numbers:
1 – report design work space;
2 – menu bar;
3 – toolbars;
4 – object's toolbar;
5 – report pages' tabs;
6 – "Report tree" window;
7 – "Object inspector" window;
8 – "Data tree" window. You can drag elements to a report page from this window;
9 – rulers. When dragging a ruler to a report page, the guide line (which objects can be adhered to) appears;
10 – status line.

2.8.1. Controls

2.8.1.1. Key control

Keys	Description
Ctrl+O	“File|Open…” menu command
Ctrl+S	“File|Save” menu command
Ctrl+P	“File|Preview” menu command
Ctrl+Z	“Edit|Undo”menu command
Ctrl+C	“Edit|Copy” menu command
Ctrl+V	“Edit|Paste” menu command
Ctrl+X	“Edit|Cut” menu command
Ctrl+A	“Edit|Select all” menu command
Arrow, Tab	Move between objects
Del	Delete of the selected objects
Enter	Call the editor of the selected object
Shift+arrows	Modify sizes of the selected objects
Ctrl+arrows	Move the selected objects
Alt+arrows	The selected object is adhered to the nearest one in the specified direction.

2.8.1.2. Mouse control

Operation	Description
Left button	Selecting an object; pasting a new object; moving and resizing objects. For the selected objects, you can perform zooming in and out by dragging the red square in the left bottom corner of the selected objects’ group.
Right button	Selected object's contextual menu.
Double-click	Object editor call. Double-clicking on the white space of a page calls the “Page Settings” dialogue box.
Mouse wheel	Scrolling a report page.
Shift + left button	Toggle object's selection.
Ctrl + right button	If you hold the left mouse button during moving a mouse, a frame appears. As soon as you release the mouse button, all the objects captured in the frame would be selected. This operation can also be performed by clicking on the blank space on the page, and moving the mouse cursor to the required position.

Ctrl + right button	If you hold the left mouse button during moving a mouse, a frame

	appears. As soon as you release the mouse button, all the objects captured in the frame would be selected. This operation can also be performed by clicking on the blank space on the page, and moving the mouse cursor to the required position.
Alt + left button	If the “Text” object is selected, it edits its contents in place.

2.8.2. Toolbars

2.8.2.1. Designer mode bar

The bar is integrated with the object bar and has the following buttons:

Icon	Name	Description
	Object selecting	A standard mode of operation, in which a cursor allows to select objects, modify their sizes, etc.
	Hand	Clicking on this icon allows dragging a report page.
	Zoom	Clicking on the left button doubles the zoom (adds 100%), while clicking the right one zooms out by 100%. When holding the left mouse button while dragging, the selected area would be zoomed.
	Text editor	Clicking on the “Text” object allows editing its contents right on the report page. If you hold the left mouse button when moving the cursor, the “Text” object appears in the selected place, and then its editor launches.
	Format copying	The button becomes enabled when the “Text” object is selected. When clicking on the “Text” object with the left button, it copies formatting, which has the previously selected “Text” object, into the object.

2.8.2.2. “Standard” toolbar

Icon	Name	Description
	New report	Creates a new blank report.
	Open report	Opens an existing report from the file. Hotkeys combination – “Ctrl+O.”
	Save report	Saves a report into the file. Hotkeys combination – “Ctrl+S.”
	Preview	Performs report constructing and its previewing. Hotkeys combination – “Ctrl+P.”

	New page	Adds a new page into the report.
	New dialogue form	Adds a new dialogue form into the report.
	Delete page	Deletes the current page.
	Page properties	Calls a dialogue with page properties.
	Variables	Calls the report variable's editor.
	Cut	Cuts the selected objects into the clipboard. Hotkeys combination – "Ctrl+X."
	Copy	Copies the selected objects into the clipboard. Hotkeys combination – "Ctrl+C."
	Paste	Pastes objects from the clipboard. Hotkeys combination – "Ctrl+V."
	Cancel	Undo the last operation. Hotkeys combination – "Ctrl+Z."
	Repeat	Redo the last cancelled operation. Hotkeys combination – "Ctrl+Y."
	Show grid	Shows the grid on the page. Grid pitch can be set in designer options.
	Grid alignment	During dragging or during modifying object sizes, the coordinates/sizes are modified step-wise, according to grid pitch.
	Locate in grid crosspoints	Modifies sizes/location of the selected objects so that they would be located at grid crosspoints.
75%	Zoom	Sets the zoom.

2.8.2.3. "Text" toolbar

Icon	Name	Description
No style	Style	Allows to select a style. To define the style list, call the "Report|Styles…" menu item.
Arial	Font	Allows to select font name from the drop-down list. Stores last five fonts previously used.
10	Font size	Allows to select font size from the drop-down list. Size can also be entered manually.
B	Bold	Enables/disables font bolding.
I	Italic	Enables/disables italics.
U	Underline	Enables/disables font underlining.
	Font	Displays Font settings dialog.
	Font color	Selects font color from the drop-down list.

	Highlighting	Shows the dialogue with highlighting attributes for the selected “Text” object.
	Text rotation	Allows to select text rotation.
	Left alignment	Enables text left alignment.
	Center alignment	Enables text center alignment.
	Right alignment	Enables text right alignment..
	Justify by width	Enables text justifying by width.
	Top alignment	Enables text top alignment..
	Height alignment	Enables text height alignment..
	Bottom alignment	Enables text bottom alignment.

2.8.2.4. “Frame” toolbar

Icon	Description	Description
	Top line	Enables/disables top frame line.
	Bottom line	Enables/disables bottom frame line.
	Left line	Enables/disables left frame line.
	Right line	Enables/disables right frame line.
	All lines	Enables all frame lines.
	No lines	Disables all frame lines.
	Shadow	Enables/disables shadow.
	Background color	Selects background color from the drop-down list.
	Line color	Selects line color from the drop-down list.
	Line style	Selects line style from the drop-down list.
1	Line width	Selects line width from the drop-down list.

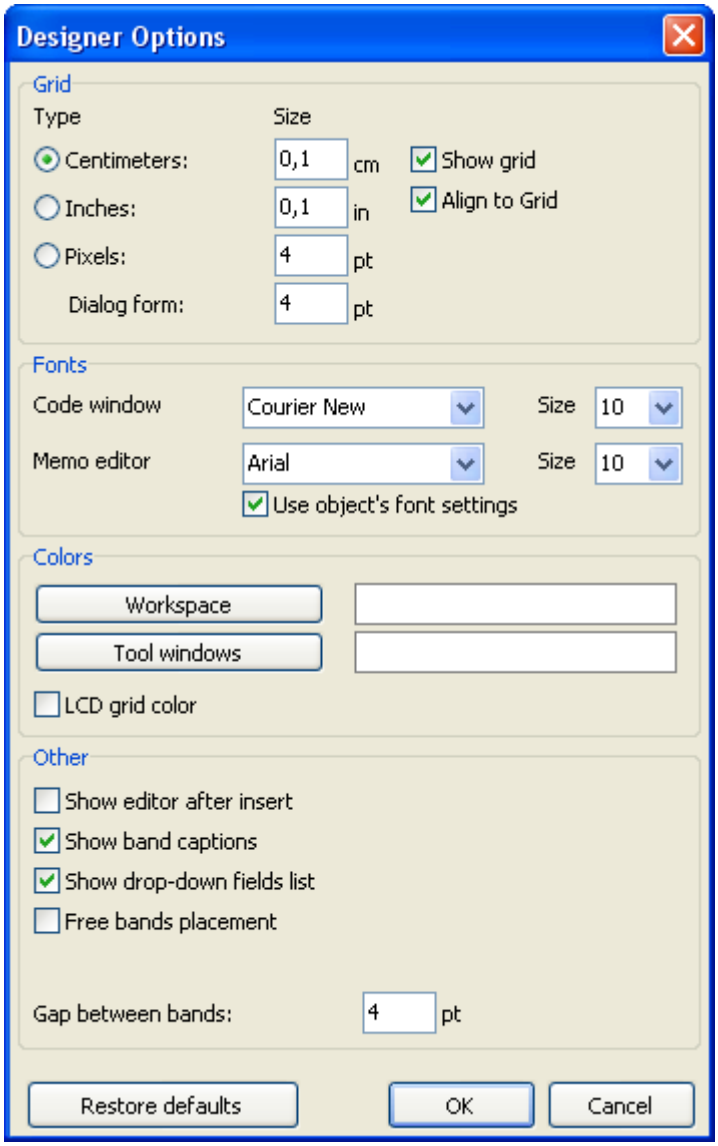
2.8.3. “Align” toolbar

Icon	Description

	Align left edges.
	Center across.
	Align by right edges.
	Align top edges.
	Justify vertically.
	Align bottom edges.
	Justify by width.
	Justify by height.
	Center across in window.
	Center vertically in window.
	Set the same width as in the first selected object
	Set the same height as in the first selected object

2.8.4. Designer options

Set the designer options via the “View|Options..." menu command.



Here you can set the desired units (centimeters, inches, pixels), and specify grid step for each unit. Tip: You can also switch units in the designer by double-clicking on the left part of the status line where the current units are displayed.

You can also specify whether grid should be displayed, and align to grid. This can be done by buttons in the “Standard” toolbar of the designer as well.

You can set a font for the code editor window and for the “Text” object editor. If the “Use object's font settings” option is enabled, the font in the text editor window would correspond with the font of the object being edited.

The default white background of the designer and service windows can be modified by the “Workspace” and the “Tool windows” buttons.

The “LCD grid color” option increases contrast of the grid lines a little, and it improves their visibility on LCD monitors.

The “Show editor after insert” option controls what happens when new objects are inserted. If the option is enabled, its editor will be displayed each time an object is inserted. When creating a large number of blank objects, it is recommended to disable the option.

Disabling the “Show band captions” option, you can disable bands’ captions in order to save some place in a page. At that, the band’s captions would be written inside of it.

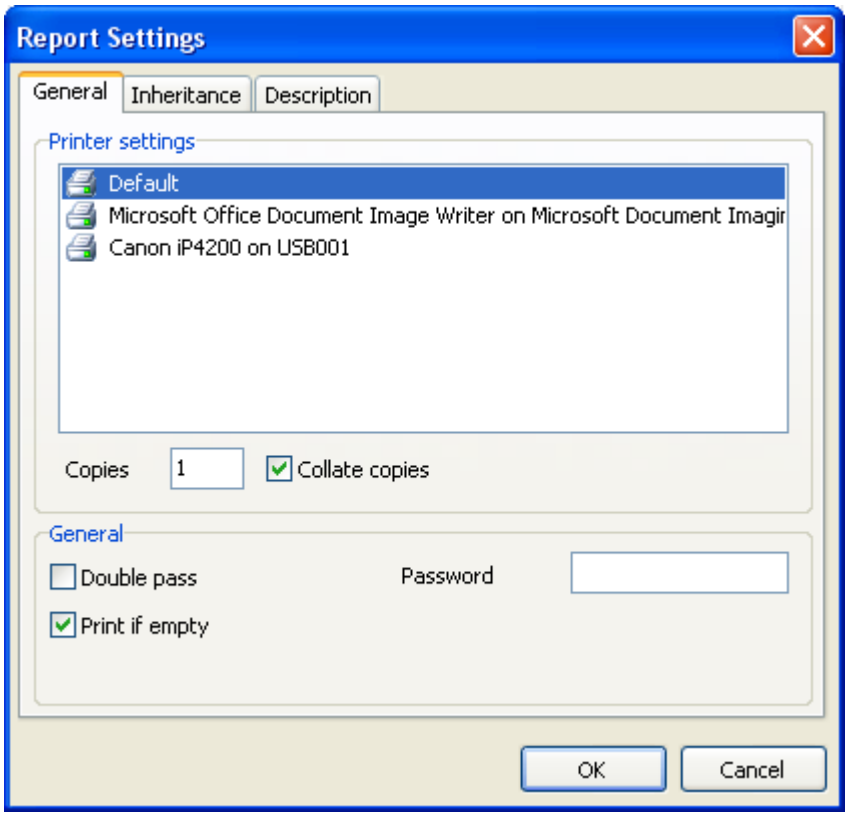
The “Show drop-down list of fields” option stops the drop-down list from displaying when pointing with the mouse to a “Text” object which is connected to data fields. This may be necessary if there are many narrow text objects in a band

The “Free band placement” option disables snapping of bands to the page. This option is disabled by default and bands are automatically grouped in page according to their function. A gap between bands can be set in the “Gap between bands” field.

2.8.5. Report settings

A window with report parameters is available from the “Report|Options...” menu. A dialogue has three pages.

In the first page you can see the general settings of the report:



You can tie a report to one of the printers installed in the system. This means that report printing will be performed by the selected printer by default. This might be useful in case when there are several different printers in the system; e.g. text documents can be tied with monochrome printer, while documents with graphics - to the color one. There is the “Default printer” item in the list of printers.

When this item is selected, the report will not be tied with any printer, and therefore printing will be performed by a printer, which is set as the default one.

You can also set number of report copies to be printed and specify, whether it is necessary to perform collation. The values, which a user sets in this dialogue, would be displayed in the “Print” window.

If the “Double pass” flag is selected, report’s formation will be performed in two steps. During the first pass, a report is formed, and is divided into pages, but the result is not saved anywhere. In the second pass a standard report formation with saving a result in the stream is performed.

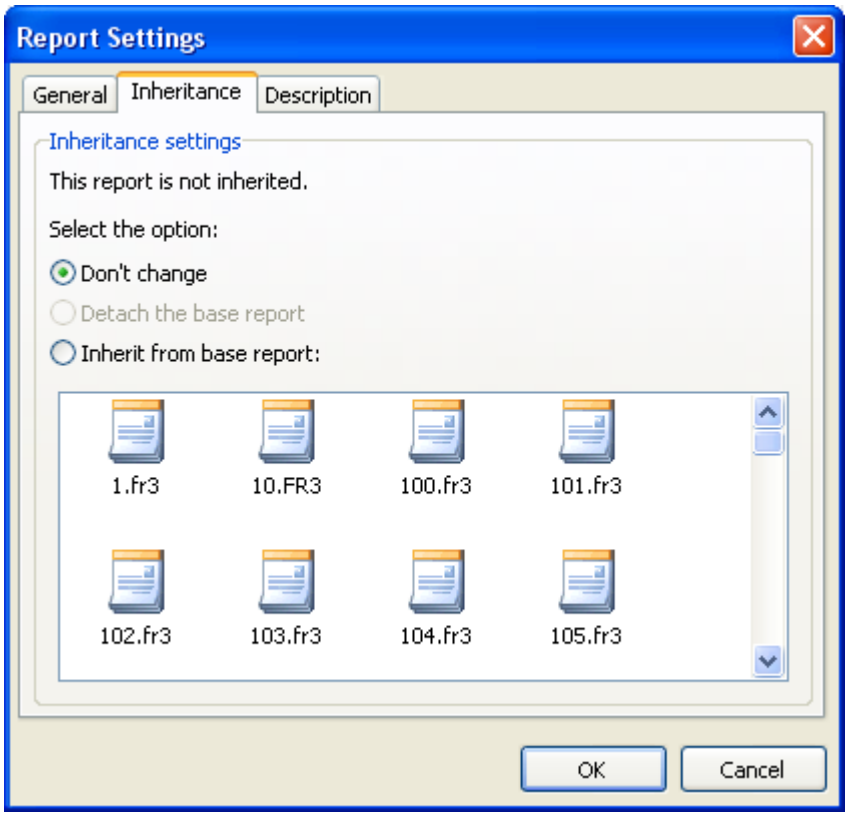
Why two passes are necessary? Most often, this option is used in cases when in a report there is a need for the total number of pages in it, i.e. the information of the “Page 1 of 15” type. The total number of pages is calculated during the first pass and is available via the “TOTALPAGES” system variable. The most frequent mistake is an attempt to use this variable in a single-pass report; in this case it returns “0.”

Another use is to perform any calculations in the first pass and display the results in the second pass. For example, when it is required to display a sum in the group header, which usually is calculated and displayed in the group footer. Calculations of this type are accomplished by writing report script code in the OnBeforePrint event of an object.

The “Print if empty” flag allows construction of a report, which contains no data lines. If this option is disabled, blank reports would not be constructed.

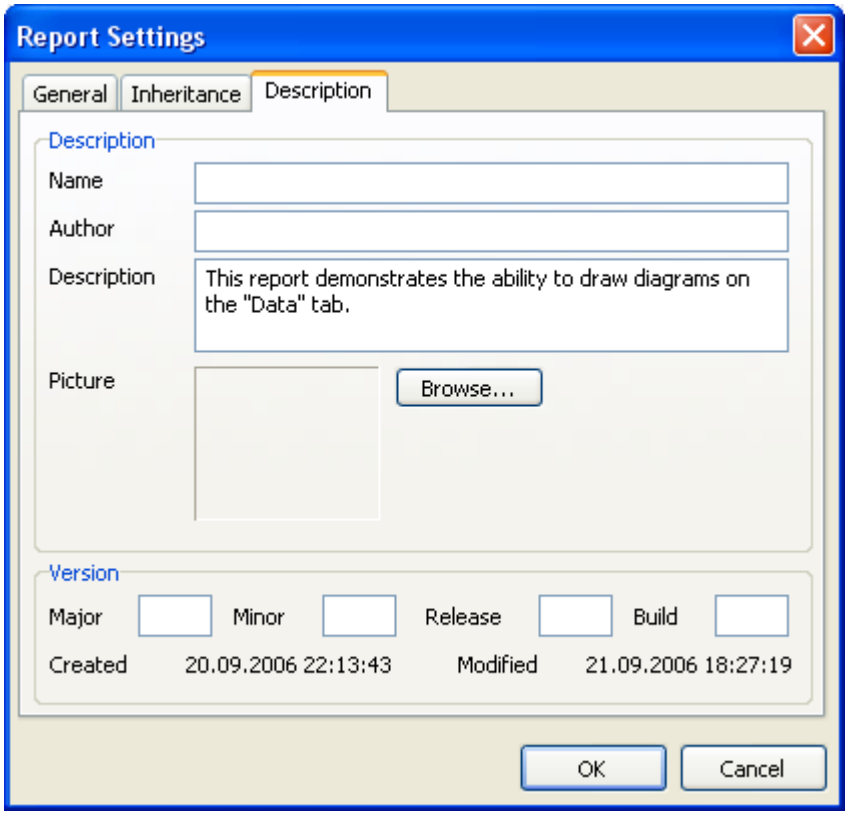
The “Password” field enables setting of a password which must be entered before opening a report.

On the second page you can setup the report inheritance options:



You can learn about inheritance later in the "Report inheritance" chapter. In this dialog you can see the base report's name (if report is inherited), detach the base report (in this case your report will be standalone, non-inherited) and inherit the report from one of base reports.

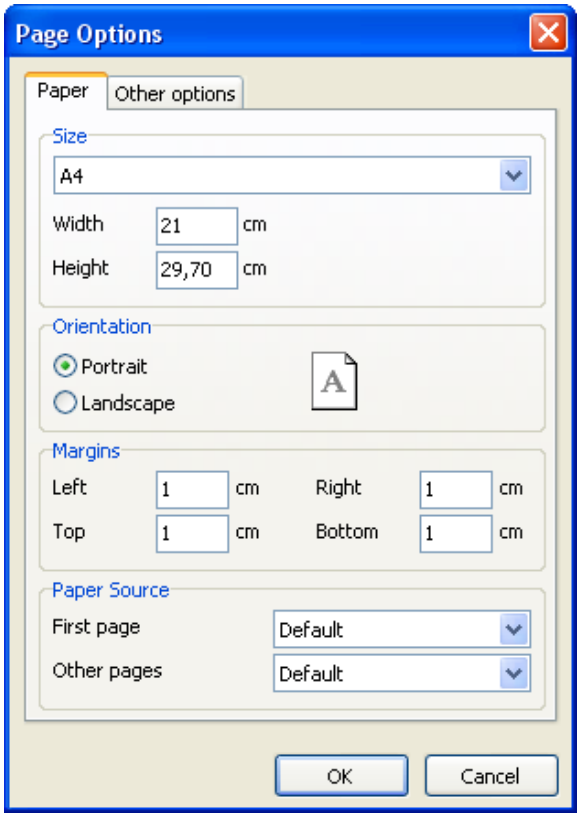
Controls in the third page of the dialogue allows you to set report's description properties..



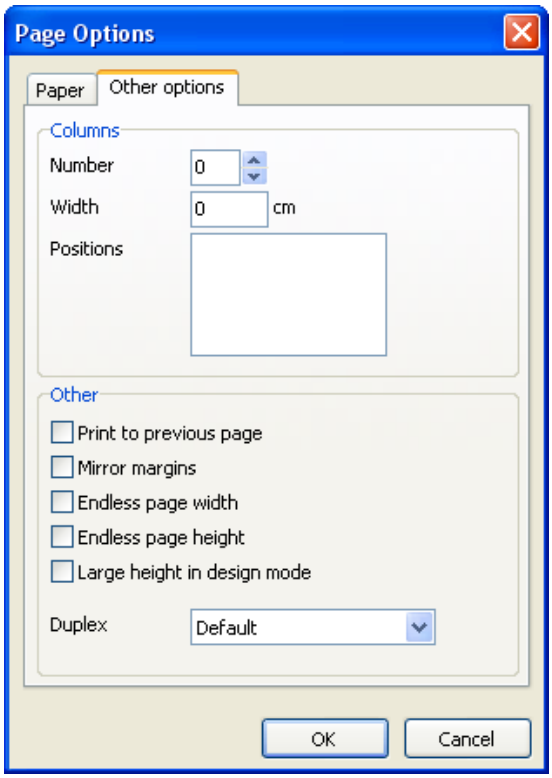
All fields in this dialog are for information purposes only.

2.8.6. Page options

Page's parameters are available via either the "File|Page settings..." menu, or by double-clicking on page blank space. The dialogue has two pages:



On the first dialogue page, you can select size and alignment of paper, as well as set margins. In "Paper source" drop-down lists you can select a printer tray for the first page and the rest of the report pages.



On the second page, you can set the number of columns for multi-column reports' printing. The current settings are displayed in the designer.

The "Print to previous page" flag allows you to print pages, beginning from blank space of the previous page. This option can be used in case when a report template consists of several pages or when printing batch (composite) reports.

The "Mirror margins" option switches right and left margins of page for even pages during previewing or printing a report.

The "Endless page width & height" option increases page's sizes depending on number of data records on the page (when running a report). In this case you will see one big page in the preview window instead of several standard size pages.

The "Large height in design mode" option increases page's height several times more. This feature can be useful if many bands are located in the page, and must be used when working with the overlay band. This only effects the page height in design mode..

2.8.7. Creating reports

2.8.7.1. Report objects

A blank report in Report Designer is presented as a paper page. At any place on the page, a user is able to add objects, which can display different information (such as text and/or graphics), as well as to define report's appearance. Let us describe briefly the assignment of the Report Designer objects, which are included in the standard package:

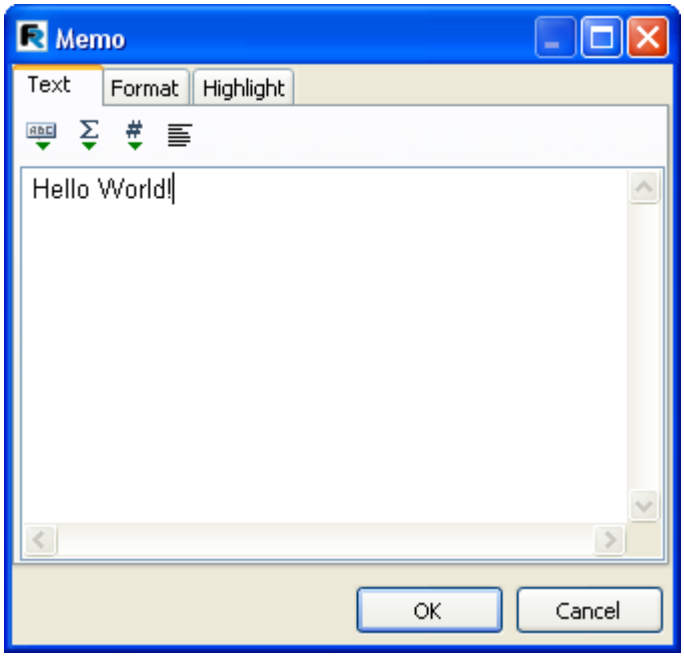
- "Band" object allows creation on a design page, of an area which has definite behaviour; according to it's type.
- "Text" object displays one or several text lines within the rectangular area;
- "Picture" object displays a graphic file in "BMP," "JPEG," "ICO," "WMF," or "EMF" format;
- "Line" object displays a horizontal or a vertical line;
- "System text" object displays service information (date, time, page number, etc), as well as aggregate values;
- "Subreport" object allows inserting an additional report design page inside the basic one;
- the objects of "Draw" category represent different geometrical figures (diagonal line, rectangle, rounded rectangle, ellipse, triangle, and diamond);
- "Chart" object displays data in the form of charts as shown on the monitor
- "RichText" object displays a formatted text in Rich Text Format (RTF);
- "CheckBox" object displays a checkbox with either a check or a cross;
- "String Grid" object displays data in the form of grid;
- "OLE" object is able to display any object using OLE technology.

The basic objects you most likely need to work with are the "Band" and "Text" objects. You will learn about their capabilities in detail further in this chapter.

2.8.7.2. "Hello, World!" report example

The report will contain one inscription only ("Hello, World!"). Open the report designer. After that, click the "Text" button in the "Objects" designer panel. Move the mouse cursor to the desired place on the page, and click again. The object has been inserted.

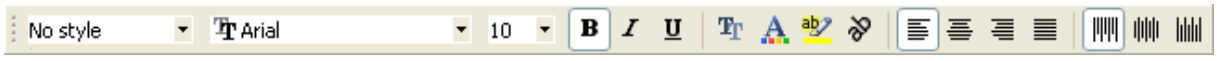
The text editor window will be displayed right away; if it does not appear (this can be set in the designer settings), then doubleclick the object. Enter the "Hello, World!" text, and then click the "OK" button.



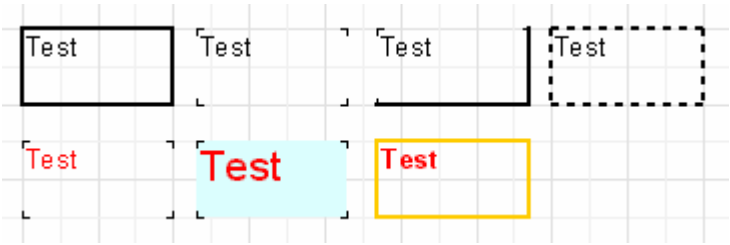
The report is created. To preview it, either select the "File|Preview" menu item, or click the corresponding button in the toolbar. The preview window containing a report page with the "Hello, World!" text will appear. This report can be printed out, saved to a file (*.fp3), or exported to one of the supported export formats.

2.8.8. The "Text" object

The "Text" object has many features. Now we already know that it allows you to display text, a frame, and fill color. The text can be displayed using any font of any size and style. All the parameters can be set visually, with the help of the toolbars:



Here are some examples of text design:

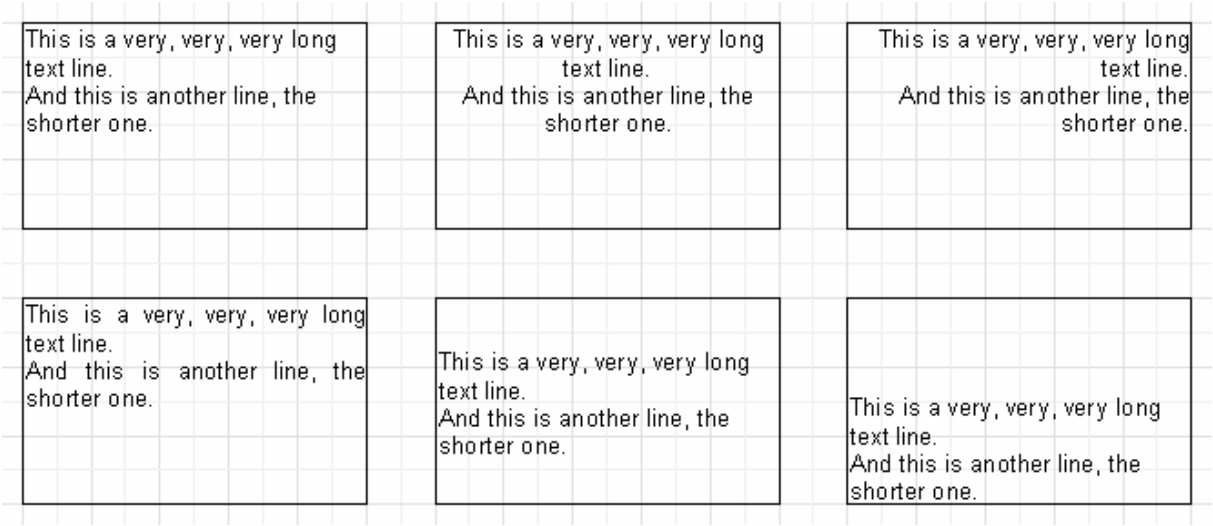


Now let's look at other features of this basic object. As an example, let us create a new text object and put two lines into it:

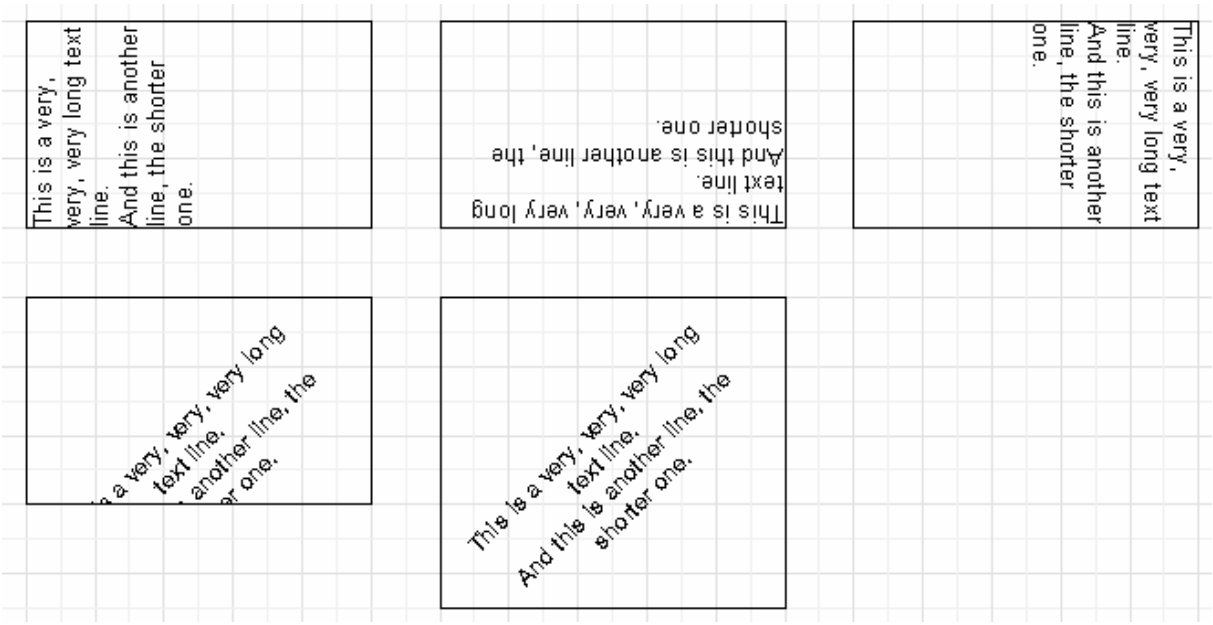
This is a very, very, very long text line.
And this is another line, the shorter one.

Let us enable the object frame, and then resize the object up to 9x3 cm with the help of the mouse. We see that the object can display not only a single line of text, but several lines as well. Now let us reduce the object width up to 5cm. It is obvious that long lines did not find room in the object and therefore were wrapped. This happens due to the "WordWrap" object property. If it is disabled (either in inspector or in the object context menu), the long lines will be simply cut off.

Now let's check how the text alignment inside the object works. Alignment buttons are located in the "Text" toolbar and allows one to set horizontal or vertical text alignment. Pay attention to the "Block Align" button; this button let's you align the paragraph on both object edges. To do this, the "WordWrap" property option must be enabled.



All the text in the memo can be rotated at any angle within the limit of 0.. 360 degrees. The button in the "Text" toolbar allows you to quickly rotate the text at 45, 90, 180 and 270 degrees. If you wish to rotate the text at any other value, use the object inspector. The "Rotation" property sets the required angle. When rotating a text, setting values other than 90, 180, 270 the text can exceed bounds of the object, as in our case (see the picture below). Let us increase object height a little, so that the text would fit the object.


This is a very, very, very long text line.
And this is another line, the shorter one.
This is a very, very, very long text line.
And this is another line, the shorter one.
This is a very, very, very long text line.
And this is another line, the shorter one.

Let us briefly examine some other “Text” object properties, which influence its appearance. Most of these properties are available in the object inspector only:

- BrushStyle – type of object filling;
- CharSpacing – space between symbols in pixels;
- GapX, GapY – text indents from object’s left and top boundaries (in pixels);
- LineSpacing – space between lines (in pixels);
- ParagraphGap – the first paragraph line indent (in pixels).

2.8.9. HTML-tags in the “Text” object

Yes, this object does understand some simple HTML tags. Tags can be located inside the text of an object. Tags are disabled by default; to enable them, either select the “Allow HTML tags” item in the object context menu, or enable the “AllowHTMLTags” property in the object inspector. Here is the list of supported tags:

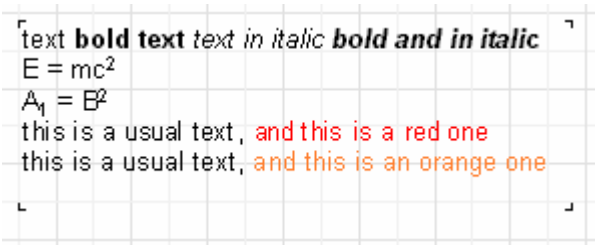
 - bold text
 - text in italic
<u> - underlined text
<sub> - subscript
<sup> - superscript
 - font color

Notice that not too many tags are supported, but it is rather enough for the majority of applications. It is impossible to modify font size and name; otherwise the text-rendering unit in Report Designer would become very complex.

The following examples demonstrate how these tags can be used.

text bold text text in italic bold and in italic
E = mc²
A₁ = B²

this is a usual text, and this is a red one
this is a usual text, and this is an orange one


text bold text text in italic bold and in italic
E = mc2
A1 = B2
this is a usual text, and this is a red one
this is a usual text, and this is an orange one

2.8.10. Displaying expressions with the help of the "Text" object

One of the most important features of this universal object is it's ability to display not only a static text, but expressions as well. Expressions can be located in the object together with text. Let us examine a simple example of how it can be performed. Put the following line into the object:

Hello, World! Today is [DATE].

Thus, when running the report, we can get something like follows:

Hello, World! Today is 01.01.2004.

What lead to such result? During Report Designer report building, if an expression enclosed in square brackets is encountered, the engine calculates it's value and inserts the value into the text (in place of the expression). The "Text" object can contain any number of expressions, together with a usual text. Both single variables and expressions can be enclosed in brackets (for example, [1+2*(3+4)]). Any constants, variables, functions, and DB fields can be used in expressions. We will learn more about these features later, in the chapter.

Report Designer automatically recognizes expressions enclosed in square brackets in the text. But what should be done if our object contains square brackets, and we do not want them to be considered as expressions? For example, if we need to display such text as following:

a[1] := 10

Report Designer considers [1] as an expression, and displays the following:

a1 := 10

that is not what we want, of course. One of the ways to avoid such a situation is to disable the expression. Just disable the "AllowExpressions" property ("Allow Expressions" in the context menu), therefore all the expressions in the text will be ignored. In our example, Report Designer would then display exactly what we need:

a[1] := 10

Sometimes text is required to contain both an expression and a text in square brackets, for example:

a[1] := [myVar]

Disabling of an expression allows us to display square brackets in the required place, but it also disables handling of expression. In this case, Report Designer allows you to use another set of symbols to designate the expression. The “ExpressionDelimiters” property, which is equal to “[,]” by default, is responsible for it. In this case, the user can use angular brackets for the expressions, instead of square ones:

a[1] := <myVar>

The “<,>” value must be set in the “ExpressionDelimiters” property. As you can see, the comma divides opening and closing symbols. There is one limitation however: the opening and closing symbols cannot be similar, so “%,%” will not work. One can set several symbols, for example “<%,%>” Thus, our example will look as follows:

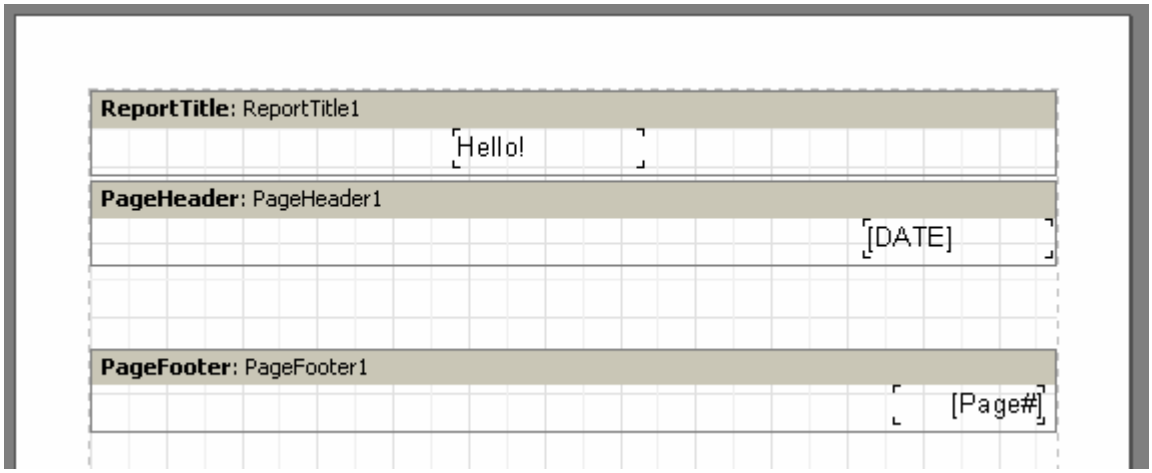
a[1] := <%myVar%>

2.8.11. Bands in Report Designer

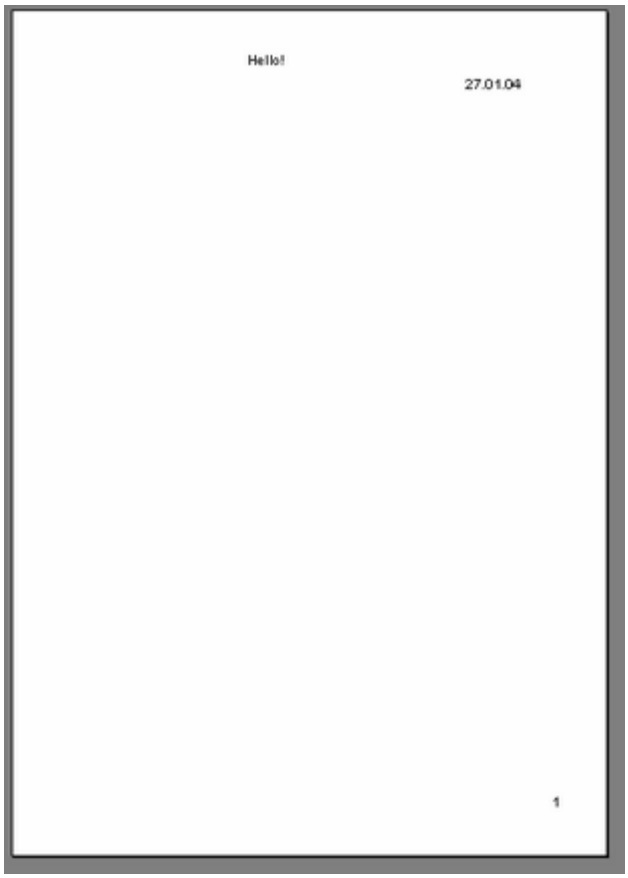
Bands are used for logically placing the objects it contains at a location on the output page. When placing an object in a band, such as “Page Header,” we tell the report engine that the given object must be displayed at the top of each page of a finished report. Similarly, the “Page Footer” band is displayed at the bottom of each page together with all the objects it contains. Let us demonstrate it with an example. We’ll create a report, which contains the “Hello!” text at the top of the page, a current date to the right of it, and a page number at the foot of the page (to the right).

Open the Report Designer designer and click the “New report” button in the toolbar. You will see a report template, which already contains three bands: “Report title,” “Master data,” and “Page footer.” Let us remove the “Master data” band for a while (to do that, click either on any free space inside the band, or on its header, and then remove it by pressing the “delete” key or using the corresponding section in the context menu). Now let us add a new band (“Page header”). To perform this, click the “Add band” button and select “Page header” from the drop down list. We see that a new band is added to the page. At the same time, the existing bands were moved down. Report Designer designer automatically positions bands on the page, and, as a result, header-bands are positioned on the top, data-bands are in the middle, and footer-bands are at the bottom.

Now let’s add some objects. Add a “System text” object in the “Page header” band and select “System variable” in its editor “[DATE]” (you should remember that the date can be displayed in a “Text” object by typing “[DATE]” in its editor). We add a “Text” object, which will contain the “Hello!” text in the “Report title” band. Note you can see, the text object, which displays page number, is already added to the “Pagefooter” band.



When running the report, you will see that the objects in the finished report are allocated on the page in the appropriate position.



Thus, bands are responsible for object positioning in required places. Depending on band type, we can add objects either at the top or at the bottom of the page, on the first page, or on the last one. The basic bands, which we would need in most reports, work in the following way:

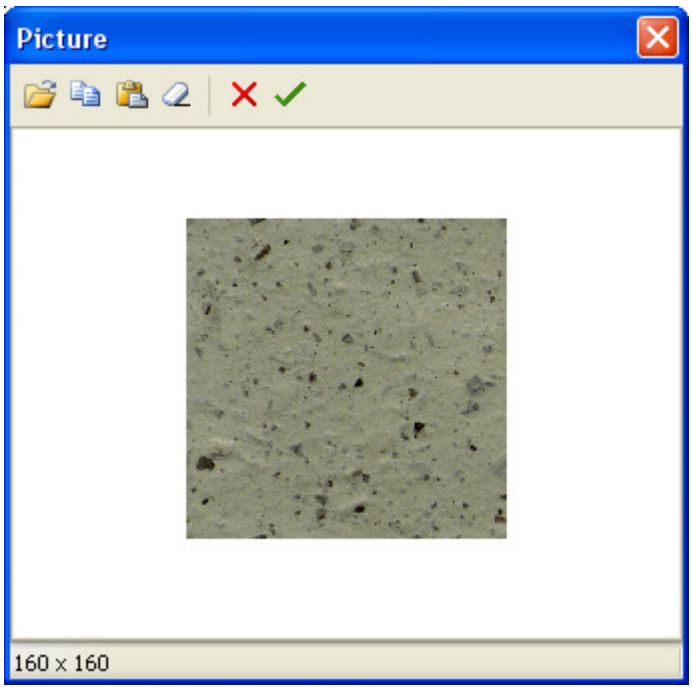
- “Page header” band is displayed at the very top of each page;
- “Page footer” band is displayed at the very bottom of each page;
- “Report title” band is displayed at the top of the first page, but below the “Page header” band (depending upon the “TitleBeforeHeader” page property assigned in the object inspector);

- “Report summary” band is displayed at the very end of a report, at white space.

2.8.12. “Picture” object

The next object to examine is the “Picture” object. It is also frequently used in reports. With the aid of this object, you can insert a logo, a photo of an employee or any other graphical information. The object is able to display graphics in “BMP,” “JPEG,” “ICO,” “WMF,” and “EMF” formats.

Let’s examine the capabilities of the object. Create a blank report and place a “Picture” object on the report page. in the object editor (if it does not open automatically, then doubleclick on the object). Load any desired picture and click “OK.” You can load a picture from a file or clear an existing picture



There are some options available in the object’s context menu, which correspond to names of the properties in the object inspector.

- AutoSize
- Stretch – enabled by default
- Center
- KeepAspectRatio – enabled by default

If the “AutoSize” option is enabled, the object will be resized, according to the size of the picture it contains. Sometimes such feature can be useful, if pictures of different sizes are to be displayed. This option is disabled by default, for convenience.

The “Stretch” option is enabled by default. This option stretches the picture inside the object. Modify the object’s size using the mouse and you will see, that the picture size always corresponds to the object’s size. If this option is disabled, the picture will be displayed in its original size. This behaviour differs from the “AutoSize” option because the object dimensions are not adjusted according to the picture size, which means that the object can be larger or smaller than the picture it contains.

The “Center” option allows aligning a picture inside the object.

The “KeepAspectRatio” option is enabled by default it stops the picture from distorting when the object’s sizes are modified. This option works only together with the “Stretch” option. Therefore, when applying any object dimensions, a drawn circle will remain a circle, without turning into an oval. The stretched picture then occupies only the part of the internal space of the object needed to display it using correct ratios. If the option is disabled, a picture will be stretched to fill the object size, and if object’s size does not correspond to the initial dimensions of the picture, it will be distorted.

Another useful property available in the Object inspector only - "FileLink". You can put a filename (c:\picture.bmp) or variable containing a filename ([picture_file]) to this property. The picture will be loaded from given filename when you run a report.

Note : If the name of the picture object is ‘Logo’ then the picture defined in the options was loaded !

2.8.13. Chart object

Mostly used in scan and kinetik methods shows this object the chart of the data.

Please select the chart by clicking the right mouse button.

2.8.14. Stringgrid object

The string grid object contains all numeric data shown as a grid table. Please select the string grid in the combobox and set the other parameters

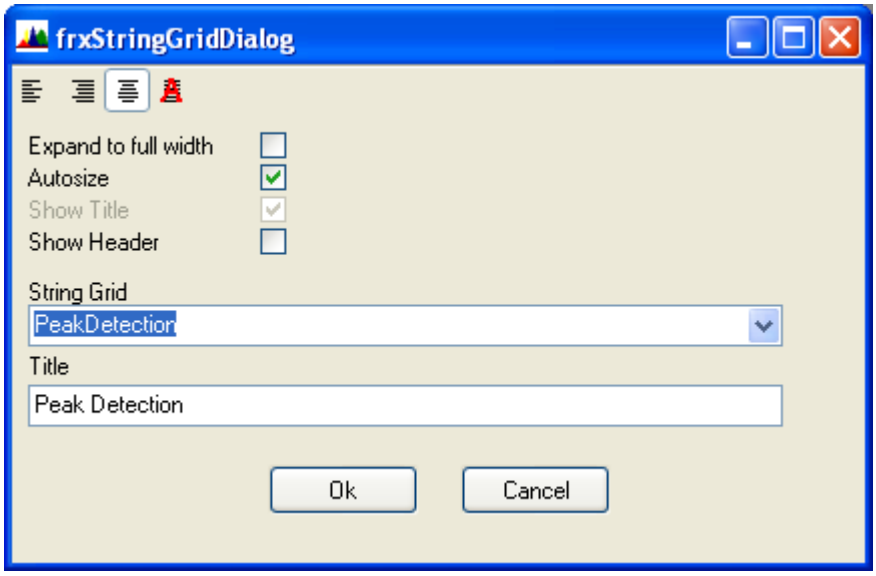
The text in the grid can be formated as left, right, center and automatic orientated. With automatic orientated the text is left orientated if it is a alphanumerical text and right orientated if it is a numeric only value.

Expand to full width : The grid was expanded to the whole width of the object, otherwise it is only equal to the calculated size of the text.

Autosize : Must be checked if expand to full width is checked

Show title : A column and row header wll be shown. Must be enabled if show header is checked.

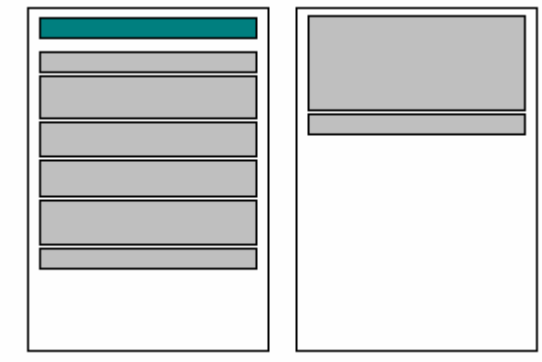
Show header : A header of he grid is visible.



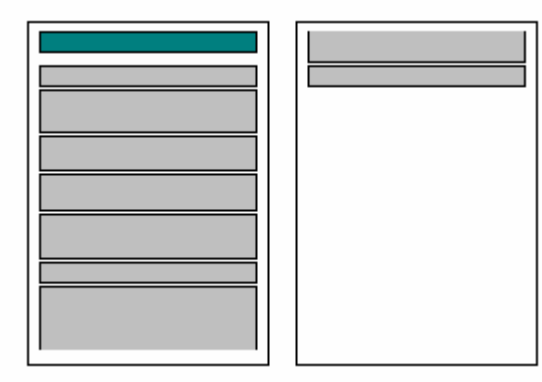
2.8.15. Data splitting

Let us pay attention to a peculiarity of this report: There is a lot of blank space at bottom of the pages. Why does it happen? When a report is constructed, the Report Designer core fills whitespace of the page with bands. After displaying each band, the current position shifts down. When Report Designer finds out that there is not enough space to display the next band (its height is larger than white space left on the page), then a new page is formed and band displaying continues there. This operation continues being performed as many times as there are records in the dataset.

Our report contains an object with large text, and that is why the band height is rather large. Furthermore, if a large band does not find room on a page, it is transferred to the next one, and much unused space remains at the bottom of the page. This is shown at the following illustration:



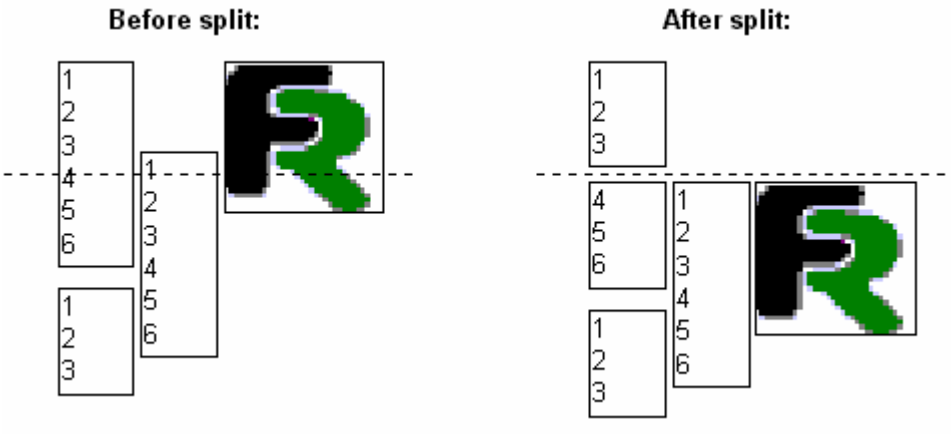
To limit paper wastage, let us use a Report Designer feature, which paragraphs the band's contents. All we need do is to enable the "AllowSplit" option of the "First level data" band. You see that there is less white space at the bottom of report pages:



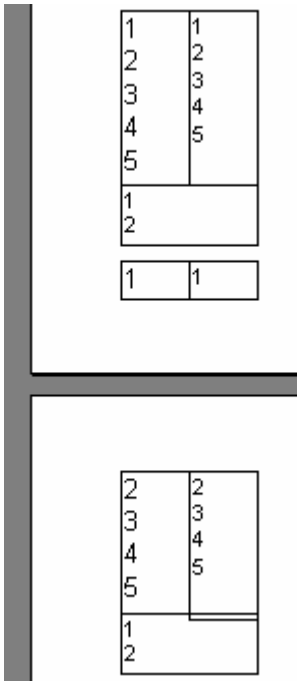
How does band splitting work? There are some objects in Report Designer, which support this feature. They are the “Text,” “Line,” and “RichEdit” objects. They can be “split,” while other objects cannot. When Report Designer comes across the need to split a band, it performs it in the following way:

- displays the non-splittable objects, which find room on white space;
- partially displays splittable objects (text objects are displayed in a way that all lines find room in the object);
- forms a new page and continues object displaying;
- if a non-splittable object does not find room on whitespace, it is transferred to the next page; at the same time, all the objects located underneath, are shifted according to need;
- the process continues until all the band objects are fully displayed.

The splitting algorithm will become clearer if to look at the illustration:



It should be noted, that the splitting algorithm is not perfect and quality of the output report may not be as expected. You should use this option very carefully in cases when objects on the split band are grouped in a complicated way, and / or their font sizes differ. Here is the example of what could be received:



2.8.16. Child-bands

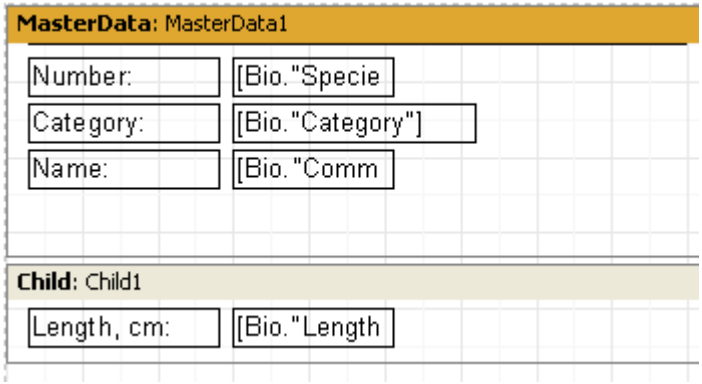
Let us examine the case when one of the lines in a report of “label” type, may have a variable size. To simulate the situation using our example, let us reduce the “Bio.”Common Name”” object width to 2.5 cm, and enable the “Stretch” option for it. Let us also enable stretching in the “First level data” band. Enable all the frame lines in all objects so that the principle of the stretching function will become clear. This will output a report with the following appearance:

Number:	90020
Category:	Triggerfish
Name:	Clown Triggerfish
Length, cm:	50
Number:	90030
Category:	Snapper
Name:	Red Emperor
Length, cm:	60

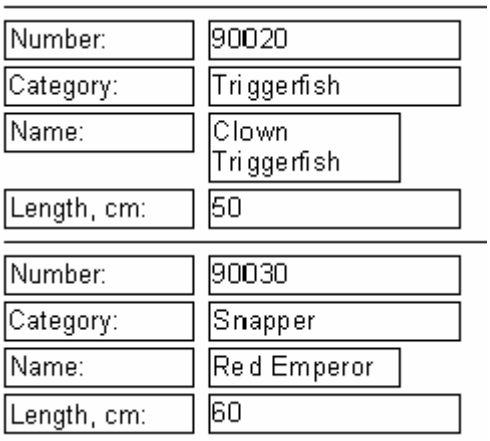
You see, that in the first case the first object contains longer text, and this is why it was stretched into two lines. Thus, the object (located underneath it and linked to the Bio.”Length (cm)” field) was shifted down. This happens because all the objects have the “Shift” property enabled by default (ShiftMode = smAlways in the object inspector). Such objects shift downwards if there is a stretchable object above

them (a “Text” object with the “Stretch” property enabled). The height value, by which the object shifts, depends on how the object from above is stretched.

However, it is unacceptable in this case, since we need the object with the “Length, cm.” text to be shifted as well. To perform this, there is a special band type in Report Designer, the “Child-band.” It is linked to (and is displayed after) it’s parent band. Add a “Child” band to our reports design layout and move the 2 Text objects into it.



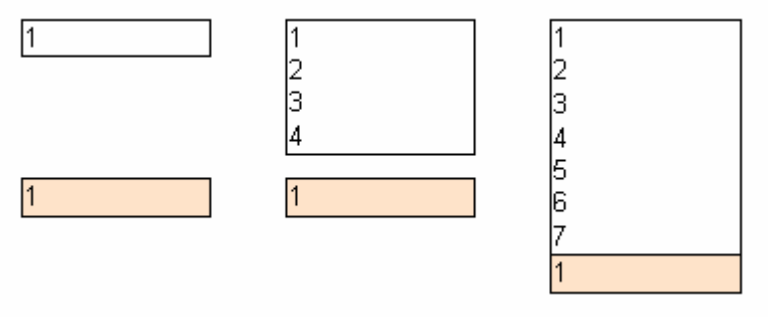
Link the Masterdata band to the Child band, by setting it’s “Child” property in the object inspector. Now, each time the “Masterdata” band prints, the “Child” band will be printed immediately afterward:



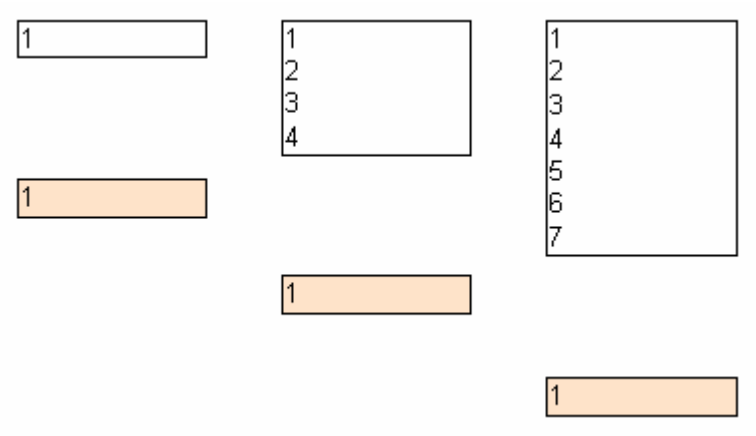
As you can see, now the title is typed exactly where it is supposed to be. In order to avoid child-band’s transferring to the next page (which basically means, it will be widowed from the parent band), enable the “Keepchild” property for the parent band (“KeepChild” in the object inspector).

2.8.17. Shifting objects

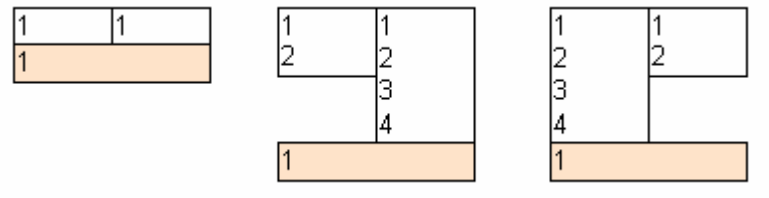
You have already seen how the “Shift” property works. Let us look at the next mode of shifting, “Shift on overlapping.” In the object inspector, the “ShiftMode= smWhenOverlapped” property value corresponds to this mode. Thus, object shifting will be performed in case, when the object from above overlaps the given object during stretching. Three cases are shown in the illustration below. As you see, the bottom object with the enabled “Shift when overlapped” option shifts only in the latter case, i.e. when there is much text in the top object and it overlaps the bottom one.



If the “Shift” option is enabled, the bottom object will be shifted anyway:



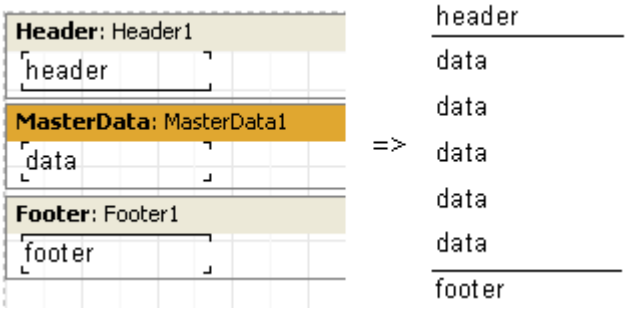
This allows one to create rather complicated report output, by using the logic of the object’s design properties, especially if an object overlaps several other objects at the same time. Thus, in the following example both of the upper objects contain stretchable texts, and the bottom one has the enabled “shifting when blocking” option. The bottom object will always be displayed closely to the object, which contains more text, irrespective of text size in the upper objects:



In this example, if the “Shift” option is enabled for this object, the bottom object will shift twice, since it is located underneath two objects and thus an unnecessary gap is formed.

2.8.18. Headers and footers of a data band

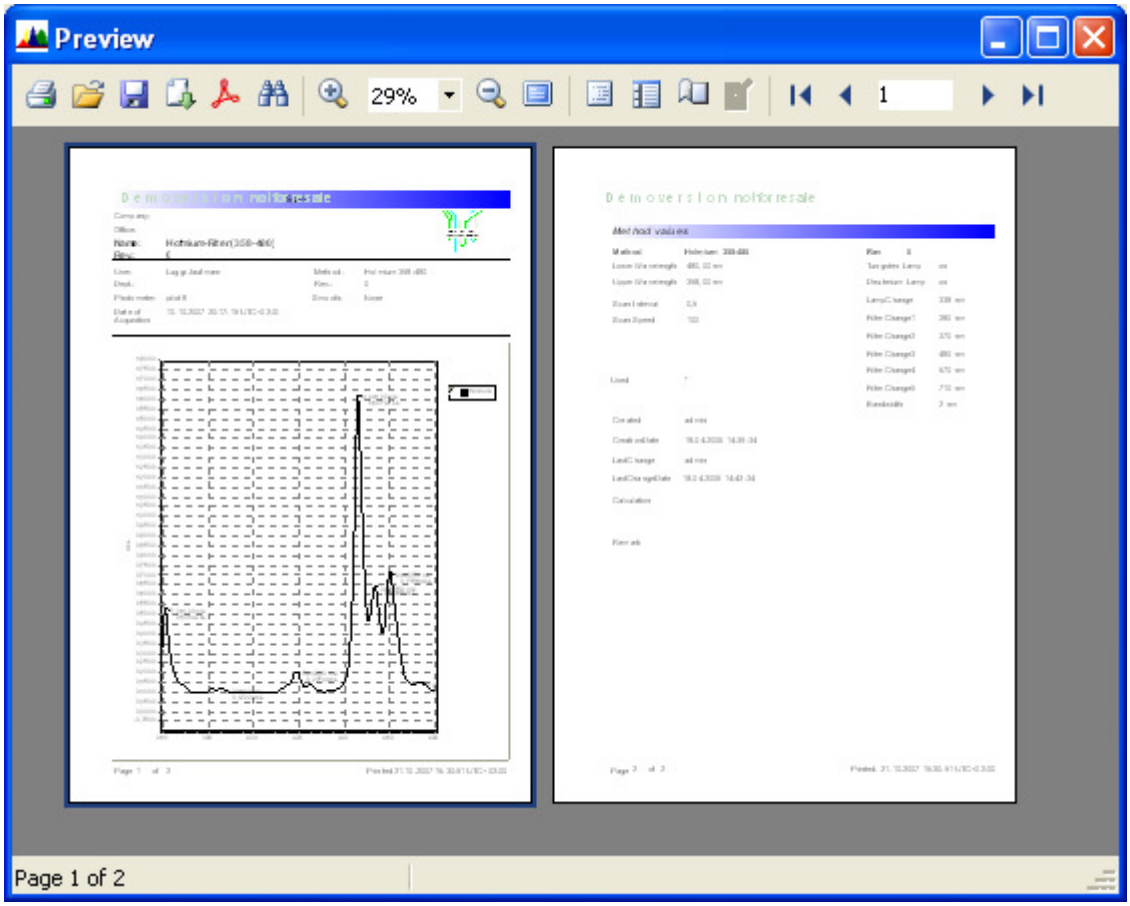
Each data band may have header and footer. Headers are output before a data band, footers are output after all data records are output. Here is an example of how the headers/footers working in case of simple report:



A simple example of title page creation. Let us use our previous report with one data level. Add a new page to it, this will be the second page. To move it to the front of the report, grab the page tab using the mouse, and then drag it to the place near the first page. At that, the pages order will be changed. Switch to the new page and place a “Text” object (with the “Our report” text inside) in the middle of the page. That is all we need to do. The report with a title page is finished.

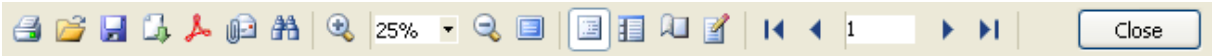
2.8.19. Report viewing, printing and export

The built report can be displayed, printed or exported into one of the supported formats. Everything can be performed in preview window.

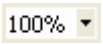
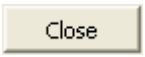


On the picture with figures the following is displayed:
1 – ready report pages;
2 – toolbar;
3 – status line;

The following buttons are on the toolbar:



Icon	Name	Description
Icon	**Name**	**Description**
	Print report	Prints report. Hotkey analogue – Ctrl+P.
	Open report	Opens file with ready report (*.fp3).
	Save report	Saves report to file (*.fp3).

	Report export	Exports report to one of the supported formats.
	Export to PDF	Exports report to Adobe Acrobat file (*.pdf). This button is displayed if corresponding export filter is installed.
	Send via e-mail	Exports report to one of the supported formats and sends it via e-mail as enclosure. This button is displayed, if corresponding export filter is installed.
	Text search	Text search in report. Hotkey analogue – Ctrl+F.
	Zoom in	Zooms in the preview.
	Scale	Selects arbitrary scale.
	Zoom out	Zooms out the preview.
	Full screen	Displays report at full screen. For returning to normal conditions perform double-click on report.
	Outline	Shows or hides the report outline.
	Thumbnails	Shows or hides the thumbnail view.
	Page properties	Calls dialogue with page properties.
	Edit page	Edits current page.
	To beginning	Transfer to the first report page.
	Previous page	Transfer to previous report page.
	Page number	Transfer to report page with pointed number. Enter number and click Enter.
	Next page	Transfer to next report page.
	To end	Transfer to the last report page.
	Close window	Close preview window.

2.8.20. Control keys

Keys	Description
Ctrl+S	Save report to *.fp3 file.
Ctrl+P	Print report.
Ctrl+F	Text search.
F3	Continue search.
Arrows	Smooth document scrolling.
PageUp, PageDown	Up/down scrolling.
Ctrl+PageUp, PageDown	Next/previous page scrolling.

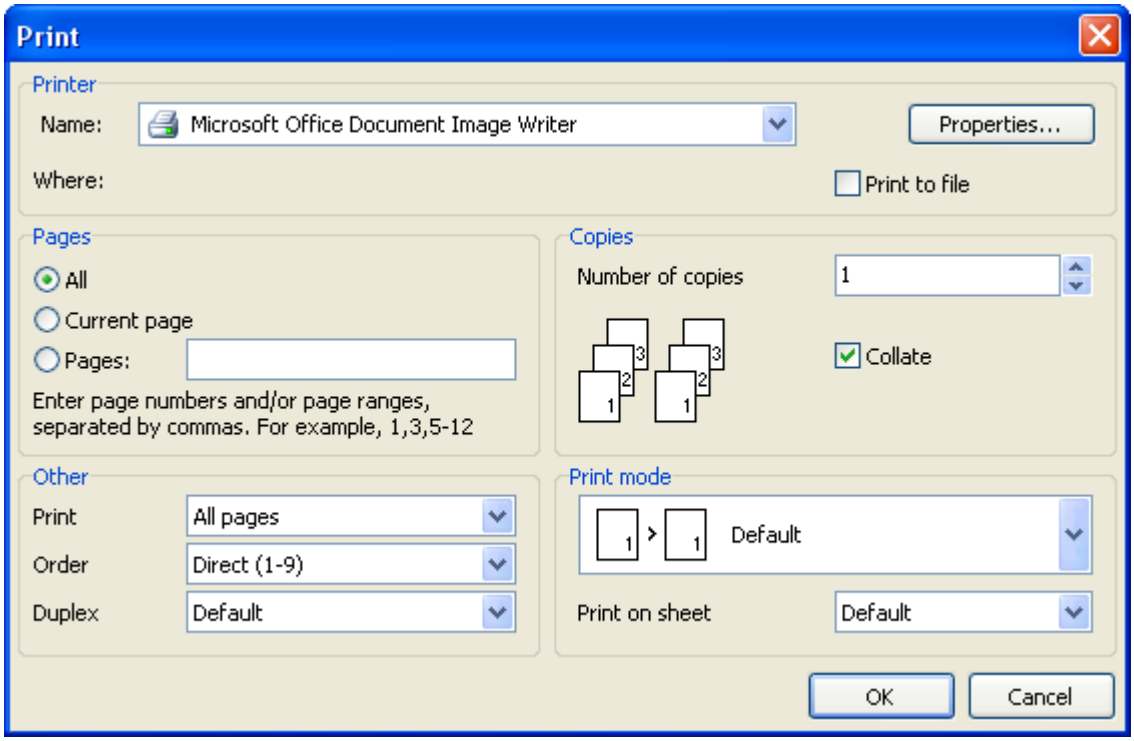
Home	Document beginning.
End	Document end.

2.8.21. Mouse control

Action	Description
Left button	Click on selected object (in interactive report); report scrolling in “hand” mode (move mouse with pressed button); zoom in is performed in “magnifier” mode.
Right button	Context menu; in “magnifier” mode zoom out is performed.
Double-click	It full screen mode it performs returning to normal conditions.
Mouse scroll	Report list scrolling.

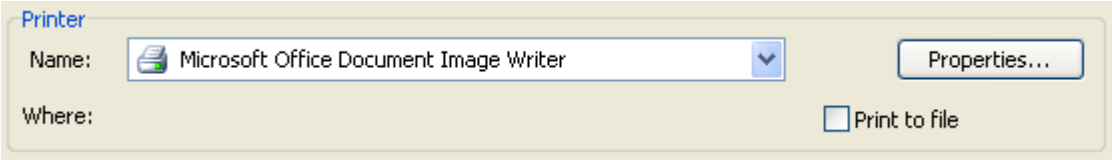
2.8.22. Report printing

To print a report click on button (or Ctrl+P hotkey). The window appears – it is printing dialogue.

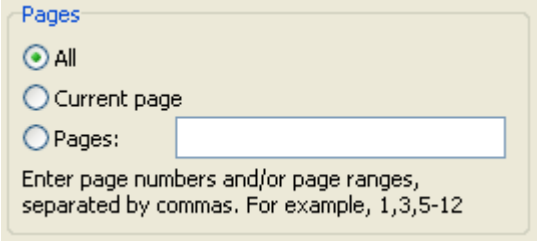


Let's look at options available in this dialogue.

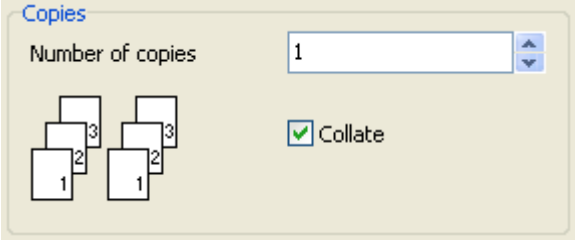
The "Printer" group: you can select a printer via which you want to print a report; set printer properties, for example, printing quality; and choose print to file.



The "Pages" group: you can select which pages to print (all, current, selected range).

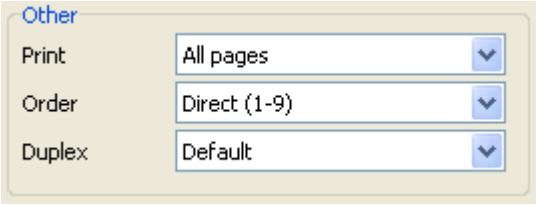


The "Copies" group: you can set how many copies to print. If Collate flag is set and you choose to print several copies, at first one report copy is printed, then – the next etc. If flag is disabled, several copies of the first page are printed, then – several copies of the second one etc.

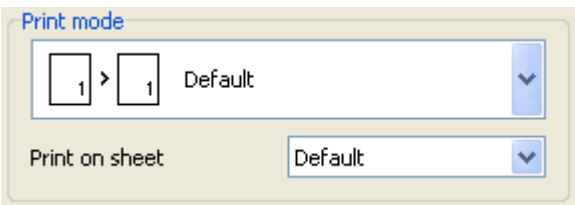


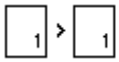
The "Other" group:

- Print - you can select which pages to print. Variants: All pages, Even pages, Odd pages.
- Order - print pages in direct or reverse order (from last to first page).
- Duplex - handle duplex by default (report settings are used) or choose one of duplex options: vertical, horizontal, simplex.

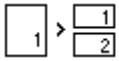


The "Print mode" group: you can select one of the printing modes.

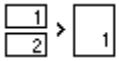



Default

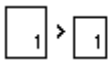
- Default mode. The printer prints on the sheet defined in a report. One preview page is printed on one sheet.


Split big pages

- Split big pages. This mode is useful if you need to print A3 report on A4 sheet. One preview page is printed on several sheets. If you choose this mode, you have to choose the sheet size ("Print on sheet") as well.


Join small pages

- Join small pages. This mode is useful if you want to print A4 report on A3 sheet. Two or more preview pages are printed on one sheet. If you choose this mode, you have to choose the sheet size ("Print on sheet") as well.

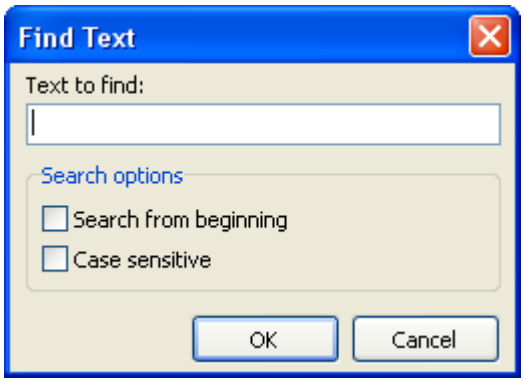

Scale

- Scale mode. Report is printed on specified sheet. All report output is scaled. One preview page is printed on one sheet. If you choose this mode, you have to choose the sheet size ("Print on sheet") as well.

After clicking on OK report printing begins. If the “Print to file” flag is selected, file name is called. And report is saved to this file (file with *.prn extension. It contains a copy of information sent to printer).

2.8.23. Text search in report

Report Designer allows to search a set text line in a text in preview window. To perform that there is button on toolbar (or its hotkey analogue - Ctrl+F). After that search dialogue appears:



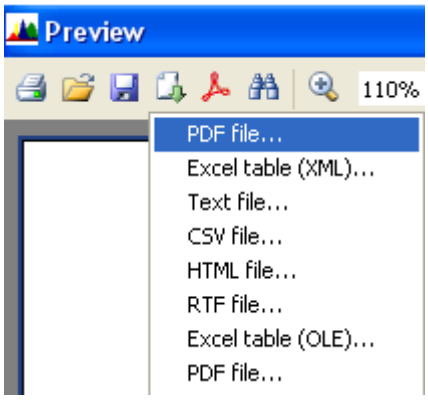
Here you can set search line and options as well:
- Search from beginning – to search text from the beginning of document. Otherwise search will be performed from current page;
- Case sensitive – to distinguish letter cases (lower-case and capital types) on searching.

On clicking OK text search is performed and the first found element is highlighted.
To continue search click F3. The following element will be highlighted

2.8.24. Report Export

Report Designer allows exporting a built (output) report to different formats for further editing, archiving, sending via e-mail, etc... To export you must add the desired FR export components to the Delphi form.

Export to 7 formats is supported. They are: PDF, Excel, XML, RTF, HTML, text, CSV. There is the ability to send report via e-mail in any above-listed formats with Report Designer means.



Exports in Report Designer use one of the following three methods:

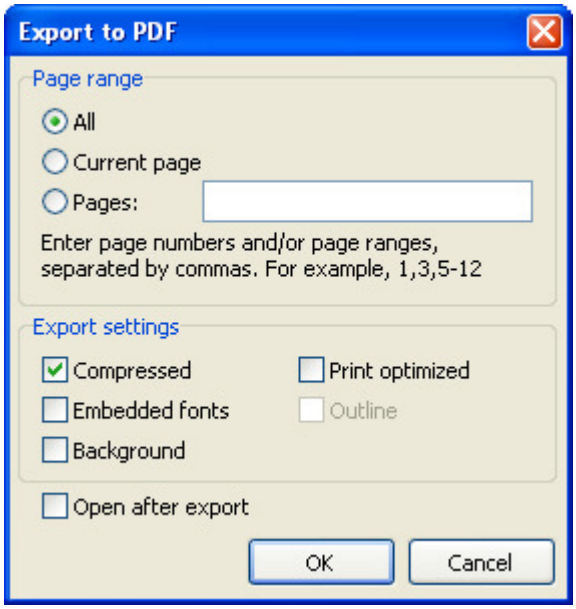
- Layer-by-layer – object transferring to resulting file is performed alternately. Expert accuracy is approximated to original;
- Table – on object transferring transitional matrix of object allocation is used. There is high accuracy to original based on the assumption that rules of creating correct report sample were followed (“Report Design References” chapter);
- Enveloping – all report objects enveloping is performed on page image. There is full original accuracy. It is used on export to graphic formats.

2.8.25. Export to PDF Format

PDF (Portable Document Format): a platform-stand alone format of electronic documents created by Adobe Systems. The free Acrobat Reader package is used for viewing. This format is rather flexible – it allows inclusion of necessary fonts, vector and bitmapped images; it allows transferring and storage of documents intended for viewing and further printing.

Export method is a layered one.

On exporting to PDF format the dialogue box for output file parameter settings appears.



Export parameters:

- Compressed – output file compressing. It reduces file size but increases export time;
- Embedded fonts – all fonts used in report will be contained in the PDF output file for correct file displaying on computers where these fonts may be absent. Output file size increases considerably;
- Background – export of graphic image assigned to a page into PDF file. It considerably increases output file size;
- Print optimized – output of graphic images in high resolution for further correct printing. This option enabling is necessary only when the document contains graphics and its printing is necessary. It considerably increases output file size;
- Outline – option is enabled when report outline is used. It enables export of the outline to the PDF document;
- Open after export – resulting file is opened right after export via PDF files viewing program which must be installed in OS by default (for example, Adobe Acrobat Reader).

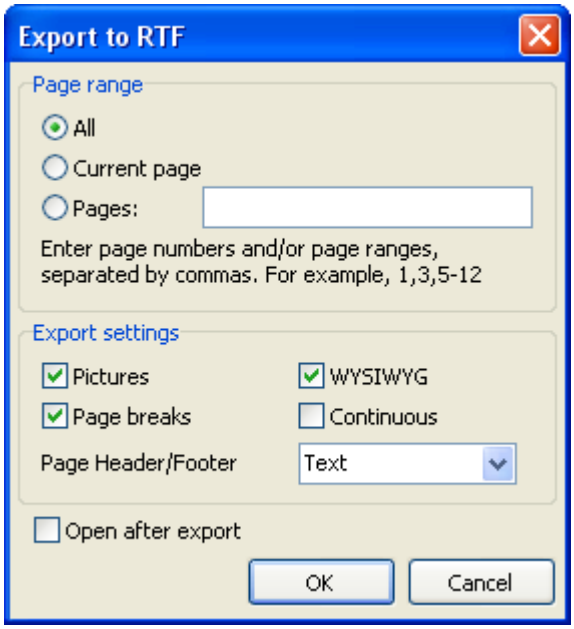
Export peculiarities: RichText objects are exported as a graphic.

2.8.26. Export to RTF Format

RTF (Rich Text Format) was developed by Microsoft as a standard for text documents interchange. Now RTF documents are supported by many modern text editors and operating systems.

Export method is a table one.

On exporting to RTF format the dialogue box for output file parameter settings appears.



Export parameters:

- Pictures – enables graphic images export to output file;
- Page breaks – enables page breaks in RTF file;
- WYSIWYG – full compliance to report appearance. Disabling the option allows optimization, reducing the number of lines and columns in the output file;
- Continuous - generate continuous document without page breaks and page headers/footers;
- Page header/footer - header/footer export mode. Variants are: Text (h/f exported as usual text), Header/Footer (h/f inserted in the document) and None (h/f are not exported);
- Open after export – output file will be opened right after export via RTF files viewing program which must be installed in OS (for example, Microsoft WordPad).

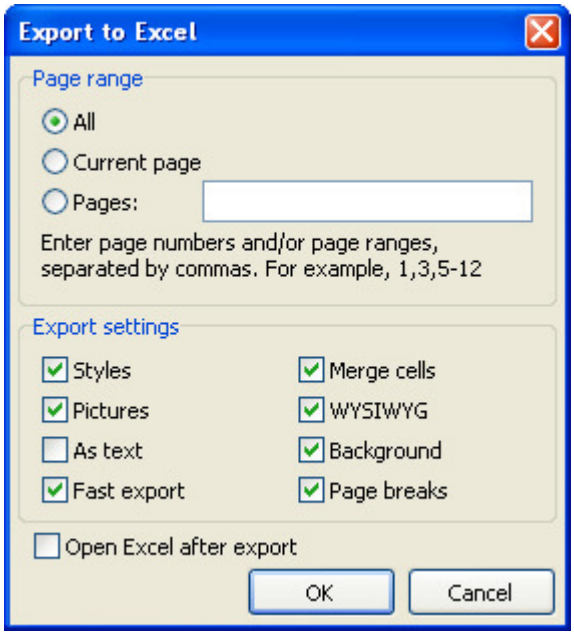
Export peculiarities: RichText objects are fully integrated into RTF format. File appearance and size depend on report sample accuracy (“Report Design References” chapter);

2.8.27. Export to Excel

Excel – application for working with electronic worksheets. It is included into Microsoft Office System.

Export method is a table/diagram one.

On exporting to Excel format the dialogue box for output file parameter settings appears.



Export parameters:

- Styles – transferring of text objects design styles into the table. Disabling increases exporting speed but worsens document appearance;
- Pictures – includes graphic images export into output table;
- As text – all objects are transferred into table/diagram as text ones. This option may be useful when transferring numeric fields with complicated formatting;
- Fast export – usage of optimized fast data transferring to Excel. This option disabling slows down data transferring but increases export compatibility on any errors during data transferring;
- Merge cells – cells integration in resulting table/diagram for achieving maximum correspondence to the original. Disabling increases exporting but reduces document appearance;
- WYSIWYG – full compliance to report appearance. On this option disabling the optimization for reducing the number of lines and columns in resulting table is performed;
- Background – export of filling color assigned to report page;
- Page breaks – includes page breaks in Excel;
- Open Excel after export – resulting file will be opened right after exporting into Excel.

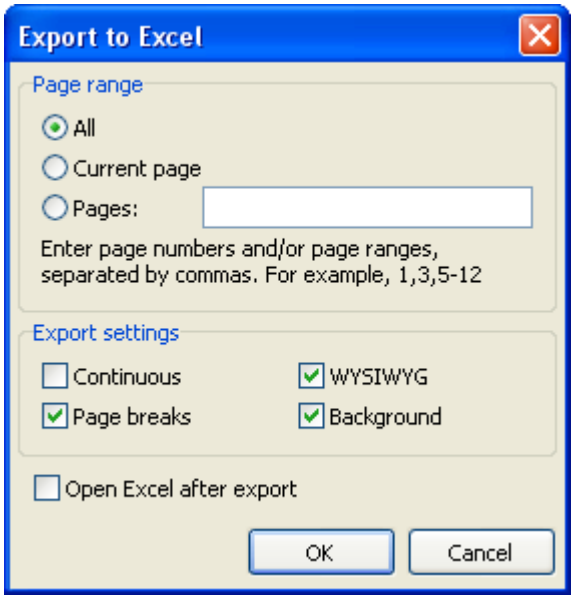
Export peculiarities: Excel program must be installed on your PC. RichText objects are transferred as simple text, graphic images transference is supported.

2.8.28. Export to XML Format

XML (Extensible Markup Language) is an expansible marking language. XML is intended for structured data storage and also for information interchange between different programs. Report Designer uses XML format for data transferring into Excel table/diagram editor ver. 2003 and later.

Export method is a table/diagram one.

On exporting to XML format the dialogue box for output file parameter settings appears.



Export parameters:

- Continuous - generate continuous document without page breaks and page headers/footers;
- Page breaks – includes page breaks in resulting document;
- WYSIWYG – full compliance to report appearance. Disabling allows reducing the number of lines and columns in resulting table;
- Background – export of filling color assigned to report page;
- Open Excel after export – resulting file will be opened right after exporting into Excel.

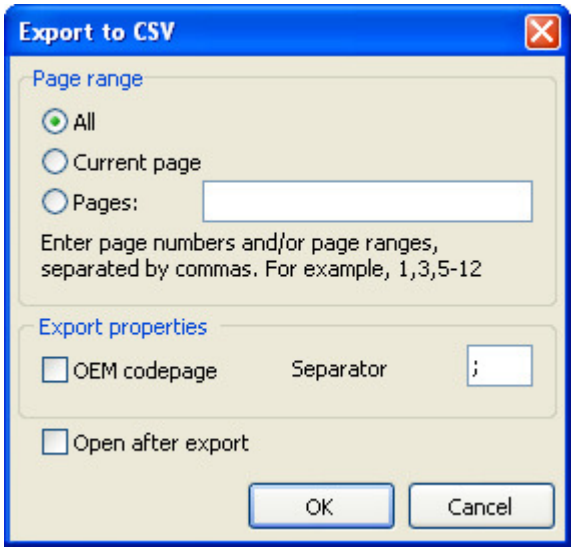
Export peculiarities: Excel program must be installed on your PC. RichText objects are transferred as a simple text; graphic images are not supported.

2.8.29. Export to CSV Format

CSV-file contains values formatted in the form of a table/diagram and adjusted in such a way that every value in column is divided from value in the next column be means of separator, and every new row begins with new line. This format may be imported into different table/diagram editors.

Export method is a table/diagram one.

On exporting to CSV format the dialogue box for output file parameter settings appears.



Export parameters:

- OEM codepage – resulting file OEM coding selecting;
- Separator – values separator in files;
- Open after export – resulting file will be opened right after exporting via CSV files viewing program which must be installed in OS.

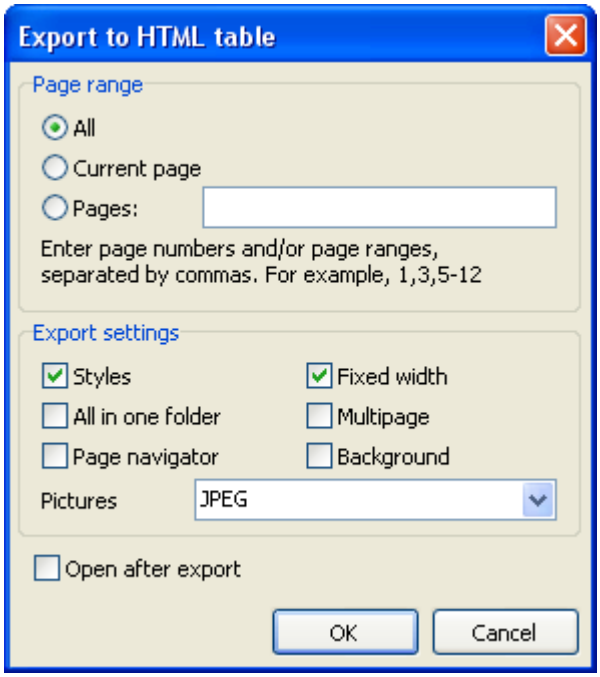
Export peculiarities: on transferring into this format report design is not saved. Graphic images are not supported.

2.8.30. Export into HTML Format

HTML (Hypertext Markup Language) is regarded as standard language for document marking in the Internet. HTML was created as a language for scientific and technical documentation interchange suitable for usage by people who are not specialists in nesting. It is used for creating relatively simple but nicely designed documents. Besides document structure simplification hypertext support is included into HTML.

Export method is a table/diagram one.

On exporting to HTML format the dialogue box for output file parameter settings appears.



Export parameters:

- Styles – transferring of text objects design styles. Disabling increases exporting but worsens document appearance;
- All in one folder – all additional files are saved in the same folder with main file;
- Page navigator – special navigator for fast shift between pages is created;
- Fixed width – blocking of automatic table/diagram width modifying on changing preview window size;
- Multipage – every page will be written to separate file;
- Background – export of graphic attributes assigned to report page;
- Pictures – includes graphic images exporting possibility;
- Open after export – resulting file will be opened right after exporting via HTML files viewing program which is allocated in OS by default.

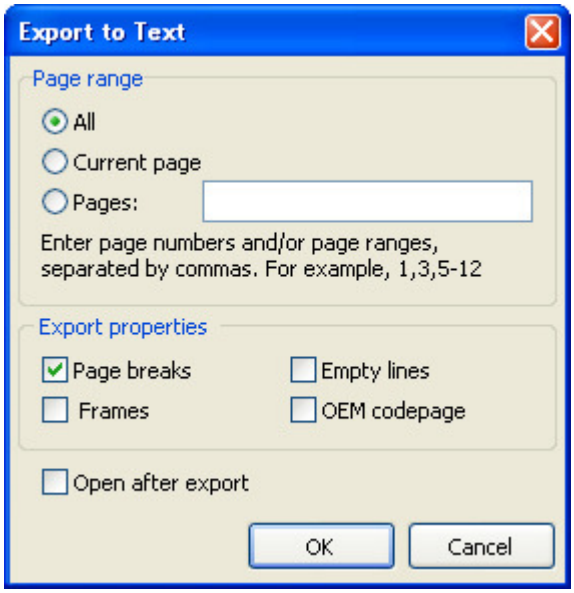
Export peculiarities: export may consist of several files. Each graphic image is supported and saved in their own separate file, RichText objects are transferred as simple text. Appearance and file volume depend greatly on report design (“Report Design References” chapter)

2.8.31. Export to Text Format

Usual text file. It contains information from report. This information is optimized to the limit and converted in accordance with the given format peculiarity.

Export method is a table/diagram one.

On exporting to text format the dialogue box for output file parameter settings appears.



Export parameters:

- Page breaks – export of page breaks to resulting file;
- Empty lines – export of empty lines;
- Frames – export of text objects frames;
- OEM codepage – resulting file OEM coding selecting;
- Open after export – resulting file will be opened right after exporting via default text files viewing program which is installed in OS.

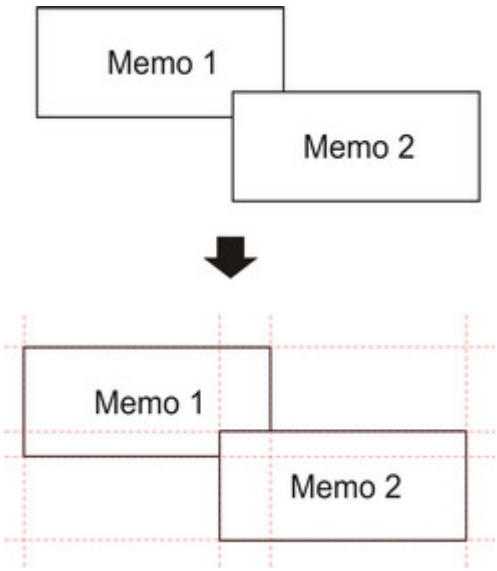
Export peculiarities: report design is not saved on transferring to this format, graphic images are not supported, exported page width is figured automatically depending on type of text objects on report page.

2.8.32. Report Design References

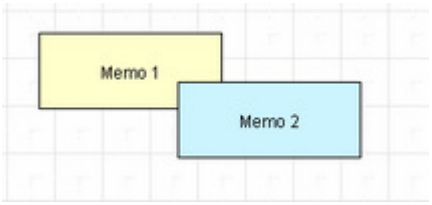
It is significant that the quality of the export into any other format depends greatly on competent design of initial report. Report Designer allows a great number of ways to manipulate objects during report output creation. This gives the advantage of fast development of any reports and their further printing. Printed document will look just as on display. And this is the primary intent of Report Designer report generator usage. The downside of such development freedom is the complexity of exporting the Report Designer document to different data formats, which have their own limits and requirements for information presentation, and are sometimes rather complex. In this chapter, special design requirements of reports intended for export to other data formats will be discussed.

Many formats use table data presentation. Formats such as HTML, XLS, XML, RTF and CSV, do. Not allow cell crossing or arranging in layers when table marking, this concerns HTML and RTF. In contrast to freedom of report development in Report Designer designer. Export filters, as a rule, take into account these requirements when objects are transferred from Report Designer report to necessary format. This is carried out by special algorithms which takes object crossings into account and their optimal placing. At object crossing points new columns and lines in the resulting output table appear. That is necessary for saving of the Report Designer transferable objects exact positioning and for getting maximum resemblance between the result and original report. A large number of cross

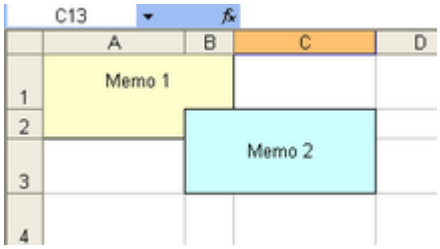
objects in report design, leads to an increased number of columns and lines in the resulting table. This leads to the need to edit the resulting file in its own editor for further use.



For example, on report design a slight crossing of two objects placed one under another on the same band. The number of records on report forming was 150. On export to RTF format 450 lines will be created (150 lines for each object and 150 ones for crossing). If we remove crossing there will be already 300 lines. In large reports and on huge number of objects the difference will be really tremendous. That, of course, will affect output file size.



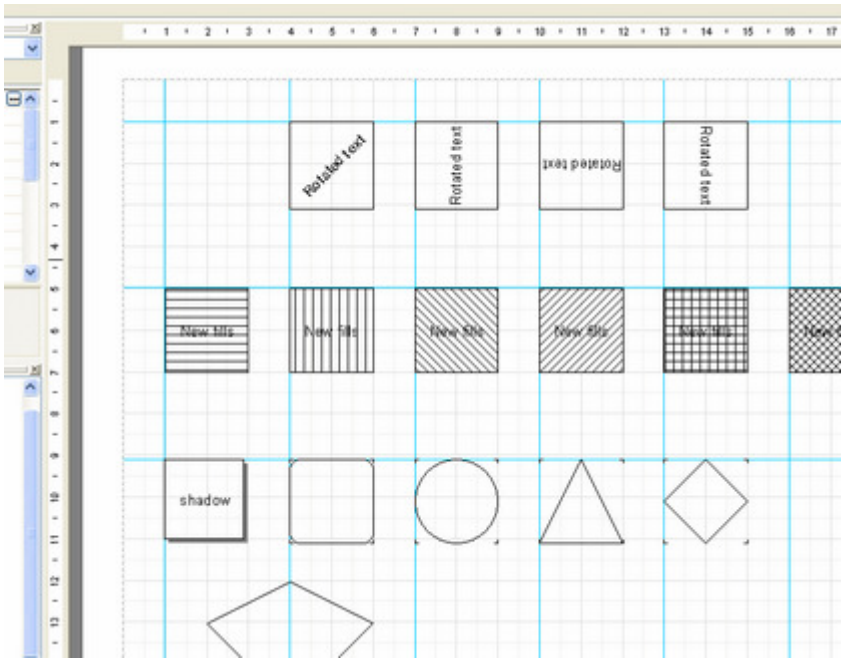
Objects in the report



Export to Excel - result

Remember that during designing, if you want to export your reports in any table format.

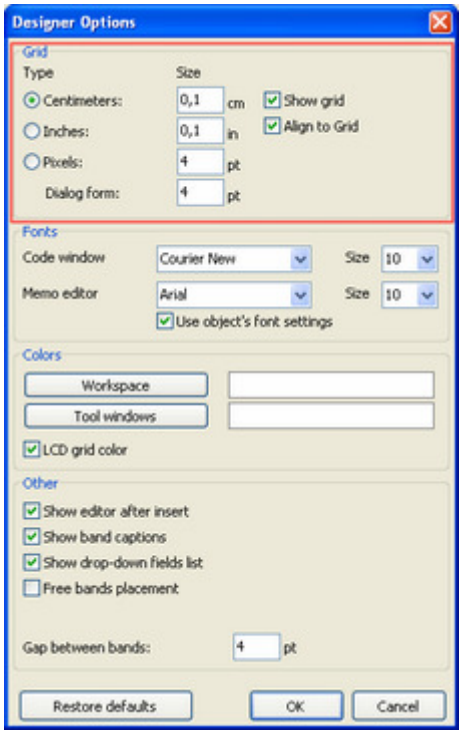
On creating tables in report keep an eye on neighboring cell's borders to adjoin each other. It is important that cells do not cross and arrange in layers. Export filter algorithm will cut off cells but export result may be far from desirable (you will see not exactly what you wanted to). Arrange objects in such a way that they are placed in line vertically as well as horizontally. Guidelines can help to perform this.



Using guidelines in the designer

To use guidelines in Report Designer designer just click on the horizontal or vertical ruler limiting report page from the left and the top. Then, holding the mouse button down, drag the guideline to the required position on the page. You will be able to place objects immediately along guidelines horizontally and vertically.

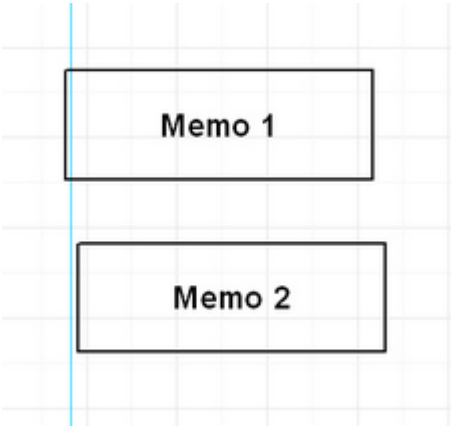
Text objects grid alignment can also be helpful in case of cells overlapping. Keep an eye on enabling grid alignment in designer options. In order to simplify alignment you can extend grid pitch. Setting of grid pitch and alignment can be found in designer menu “View” – “Options” – “Grid”.



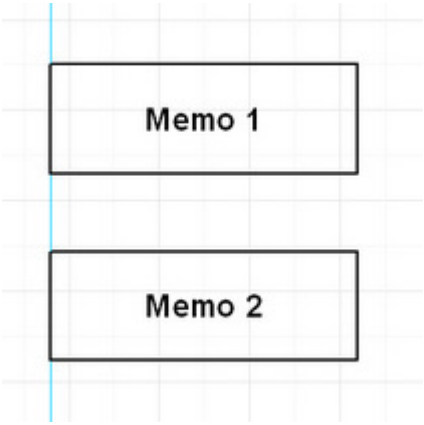
For text framing it is better to use text object embedded properties instead of single graphic objects – lines, rectangles, etc. try not to use background objects under transparent text objects.

Keeping these simple rules in mind will help you to create a report which will look perfect after export to any format using table (or table-based) marking for data presentation.

Below there are some examples of correct and undesirable object arrangement on report design creation.

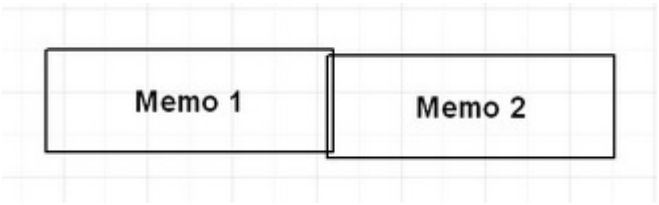


Bad

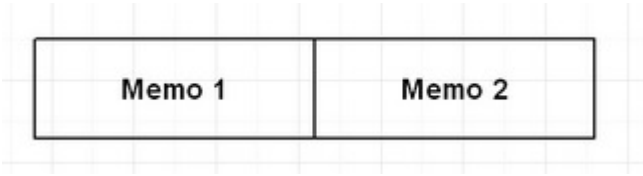


Good

Objects are displaced horizontally. It is necessary to use alignment according to extension lines as far as possible for objects to have the same horizontal coordinate.



Bad



Good

Objects are overlapping. In such a case on export to table/diagram format additional useless lines and columns and also 3 additional cells in crossing zone are created.

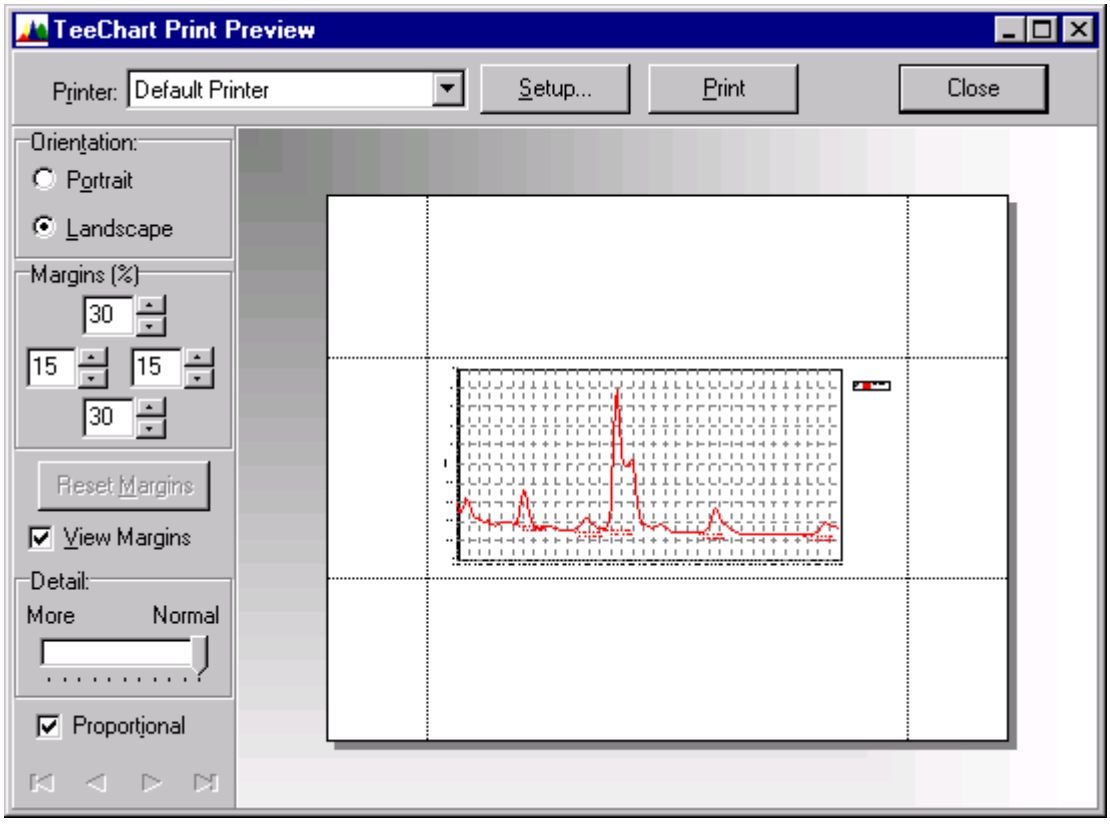
It is recommended to get acquainted with demo reports included with the Report Designer installation for mastering basic methods of optimum report development.

2.9. Managing curves

2.9.1. Direct Printing of Curves

Clicking on the *Chart* tab in the *Report* screens of modes such as *Wavelength Scan* gives the user a direct full screen display of the curves corresponding to the selected report. The appearance of the curve may be modified using the *Edit* function which is described in a separate section below.

Prints the curve as a single sheet report. Click on this icon to obtain the formatting window below. This method will only print the curve itself.



The upper bar in this dialogue box controls the actual operation and selection of the printer parameters using the standard printer installation windows.

The left-hand section of the window contains formatting functions which directly influence the print-out itself, e.g. margins, detail etc. Changes to these parameters directly influence the appearance of the print-out preview in the dialogue window. These functions are explained briefly below:

Orientation Selection of either landscape (horizontal) or portrait (vertical) format for the print-out.

Margins Spin selection boxes allow direct setting of the individual page margins.

Reset Margins Changing the preset margins automatically activates the *Reset Margins* button, click on this at any time to reset all margins to their default values. The button is not active if the margins are already set to their default values.

View Margins This checkbox allows the margin display in the preview to be switched on or off as required.

Detail Moving the scroller between normal and more increases the degree of detail shown in the curve display print-out. For example, for greater detail on the axis display move the cursor towards more until the required detail is displayed.

Proportional This returns the print-out to its original default settings without affecting the detail selected in the detail scroll bar.

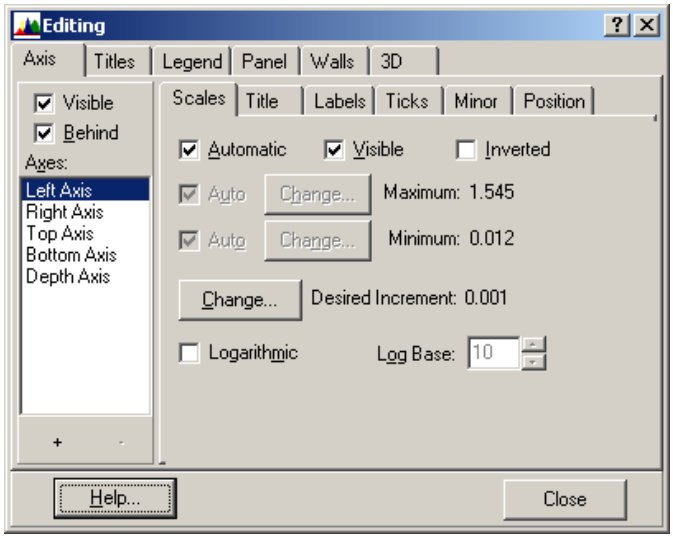
2.9.2. Editing and Formatting of Charts

The software uses a built-in editor which offers comprehensive formatting capabilities for both 2D and 3D reports. Access to this editor is obtained by clicking on the *Edit* icon. This icon is available in all screens including the *Acquisition* screen. Use of the *Edit* facility when programming a method allows immediate control of the appearance of the result without the need for time-consuming manual manipulations.

A *Help* function is provided within the *Editor* and therefore this document will only describe the more common needs with respect to formatting of charts, the user is referred to the *Help* function for additional information.

2.9.2.1. Changing the scaling (Axis)

The axis scaling is the first available tab in the *Edit* dialogue box when opened. Separate parameters can be defined for each axis and normally users would only be concerned with the so-called left and bottom axes (Y and X respectively).



The required axis to be formatted is selected by clicking in the list in the left-hand panel. Above this panel there is also a checkbox which allows the axes to be removed from the chart (visible or not). The significance of the other parameters is described briefly below:

2.9.2.1.1. Scales

Automatic The software uses dynamic scaling depending on the level of the signal obtained. In many cases this can be confusing for the user and generally it is recommended that, once known, the range should be set manually for routine operation.

Visible Check this box if you want an axis to be visible, uncheck to remove it.

Invert Checking this box will invert the chart.

Maximum If automatic is set to off, a fixed signal maximum can be defined here.

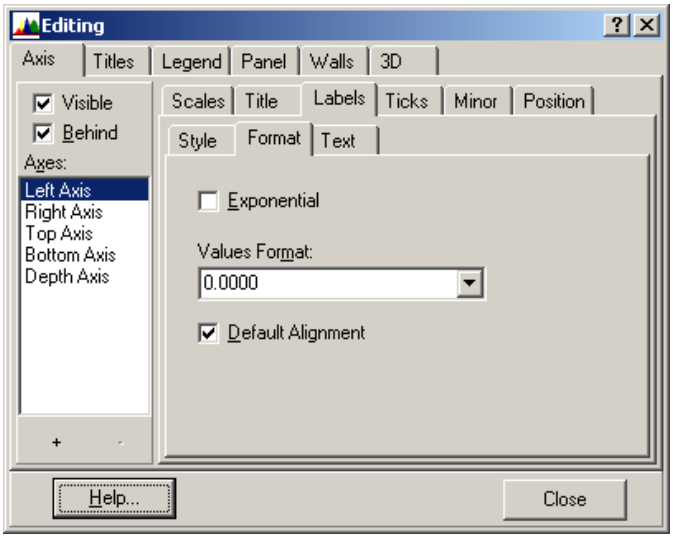
Minimum If automatic is set to off, a fixed signal minimum can be defined here.

Desired increment The desired axis increment is the minimum step between axis labels. It must be either a positive number or DateTime value. This value will be used as the initial step value. If there is not enough space for all labels, then a larger increment will be automatically calculated.
This value defines only the increment used on the scale, it is also possible to format the number of decimal places required as described below.

Logarithmic Check this box to obtain a chart based on the corresponding logarithm.

2.9.2.1.2. Decimal Format

The decimal format required can also be set from within the *Axis* tab. Click on *Labels* and then on the *Format* tab to obtain the following window:



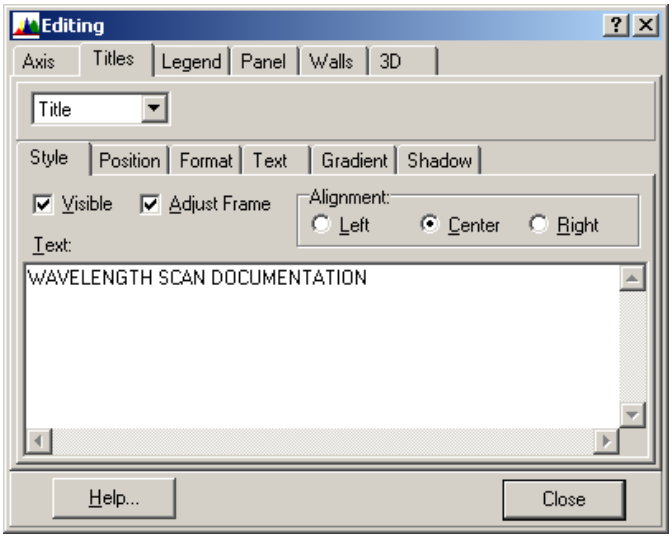
Enter the required decimal format in the “Values Format” box, e.g. for 4 decimal places enter “0.0000”.

2.9.2.1.3. Title

This allows formatting of the name to be used for a given axis, e.g. Absorbance. The tabs allow definition of the name, its alignment relative to the axis and also the font and test appearance to be used.

2.9.2.2. Titles

Normally only the definition of a chart titles in the form of either header or footer text is required. This can be done by selecting the required function using the drop-down menu and entering the text in the lower panel.

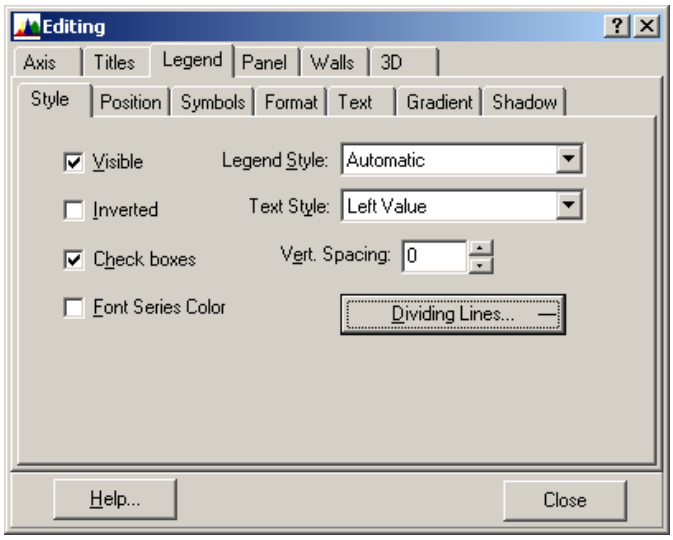


Alignment top or bottom is dependent on this selection while the horizontal position can be controlled directly from the *Alignment* box. A custom alignment using coordinates is also possible by clicking on the *Position* tab.

The remaining tabs are used to define the font type, colours, frame and certain special effects such as shadowing etc.

2.9.2.3. Legend

The legend box is used to show which curve colour corresponds to a particular sample. The default text used is “Series N” where N is the number of the sample in the batch. This default text is only used when no sample description is defined otherwise the actual description will be used automatically for the legend.



The *Style* and *Position* tabs are most likely to be used. The remaining tabs control items such as size and form of the displayed symbol and generally the applied default values will not need changing.

2.9.2.3.1. Style

Visible — Unchecking this checkbox will remove the legend box from the chart.

Inverted — Checking this box will cause the legend order to invert, i.e. the last sample to run will be shown at the top of the box.

Checkboxes — Unchecking this box will remove the checkboxes adjacent to the text in the box. This is not recommended since the checkbox is very useful if a single curve should be removed from the overlay for any reason.

Legend Style — It is recommended to maintain this setting as Automatic per default.

Text style — It is recommended to maintain this setting as Left Value per default.

Vert. Spacing — Controls the line spacing used within the legend box.

Dividing Lines — Allows definition of the format of lines used between the individual legend entries within the box.

2.9.3. Audit Trail

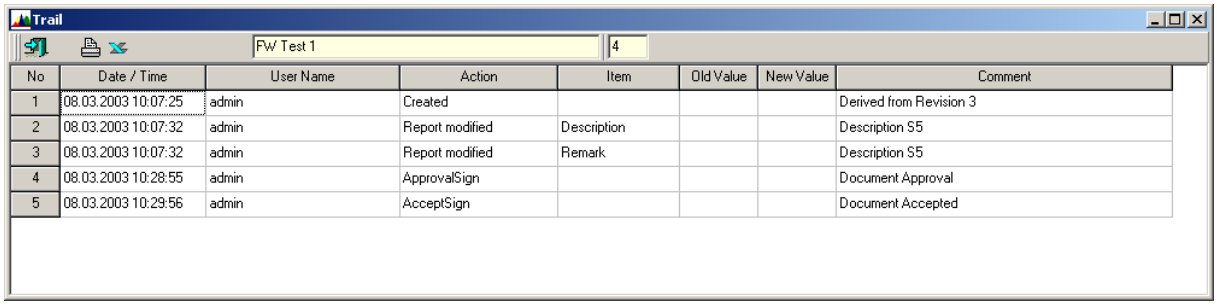
The UVS software contains an integrated *Audit Trail* which tracks all changes made to all documents after acquisition. This trail is applied to both methods and all reports and is linked to name and revision of a document.

Click on the *Audit Trail* icon in any screen to view the audit trail window for the current document and revision.

A prompt will appear asking whether you wish to view the “Report Trail”, which contains the current reports, or “Deleted Reports”, which contain audit trails for all deleted reports.

It is possible to print a report of the highlighted trail by clicking on the print icon in the top menu bar or alternatively the trail can be exported directly to Excel if required.

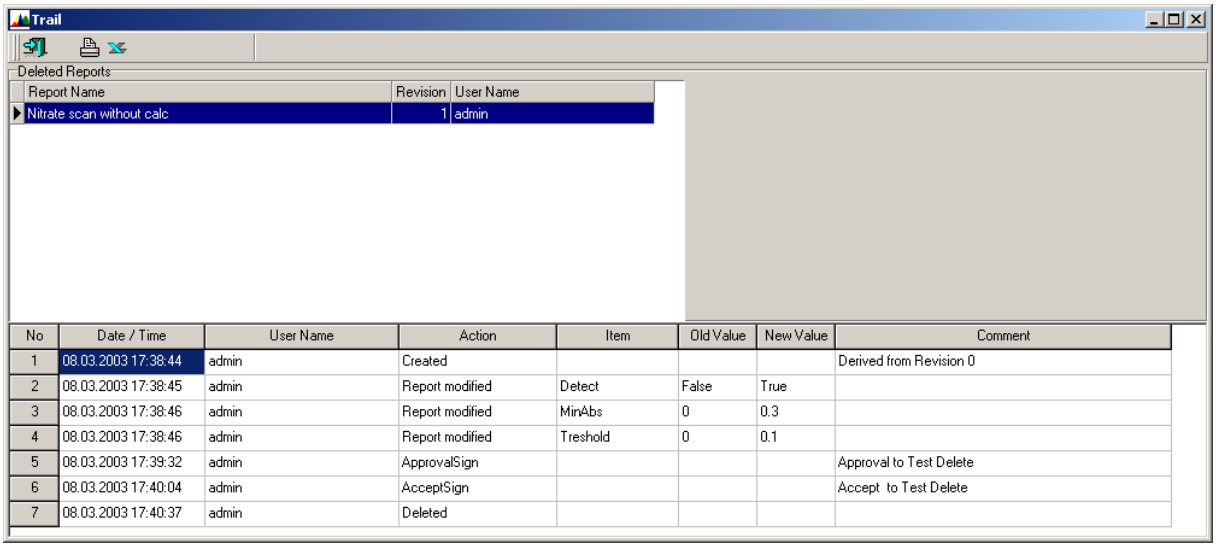
2.9.3.1. Report Trail



No	Date / Time	User Name	Action	Item	Old Value	New Value	Comment
1	08.03.2003 10:07:25	admin	Created				Derived from Revision 3
2	08.03.2003 10:07:32	admin	Report modified	Description			Description S5
3	08.03.2003 10:07:32	admin	Report modified	Remark			Description S5
4	08.03.2003 10:28:55	admin	ApprovalSign				Document Approval
5	08.03.2003 10:29:56	admin	AcceptSign				Document Accepted

2.9.3.2. Deleted Reports

The deleted report trail screen is obtained by clicking on the deleted report selection:



Report Name	Revision	User Name
Nitrate scan without calc	1	admin

No	Date / Time	User Name	Action	Item	Old Value	New Value	Comment
1	08.03.2003 17:38:44	admin	Created				Derived from Revision 0
2	08.03.2003 17:38:45	admin	Report modified	Detect	False	True	
3	08.03.2003 17:38:46	admin	Report modified	MinAbs	0	0.3	
4	08.03.2003 17:38:46	admin	Report modified	Treshold	0	0.1	
5	08.03.2003 17:39:32	admin	ApprovalSign				Approval to Test Delete
6	08.03.2003 17:40:04	admin	AcceptSign				Accept to Test Delete
7	08.03.2003 17:40:37	admin	Deleted				

The upper panel contains those reports contained in the list, by clicking on one of the reports the detail for that highlighted report is shown in the lower panel.

2.9.4. Electronic Signature

The UVS software supports an electronic signature process as required under the CFR21 Part 11 Rule.

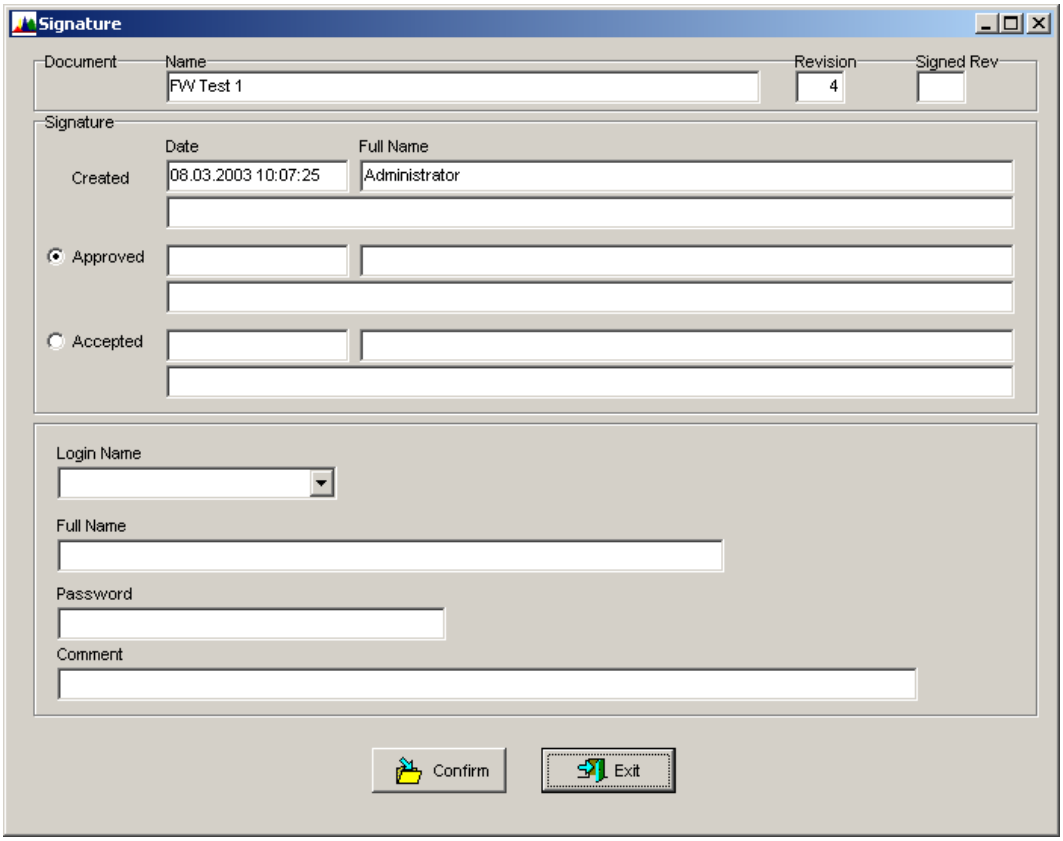
2.9.4.1. Signing a Report

In order to sign a report the signee must have been assigned the correct permission rights for the required action.

E.g. In order to be able to approve a document the user must have been assigned *Approver rights* by the administrator in the *Login* screen.

Reports can be signed even though the signees are not actually logged into the system at the time. Entry of the password is however mandatory for acceptance of any signature for *Approval* or *Acceptance* of a document.

Click on the *Signature* icon to open the following dialogue window for signing a document:



The process of signing is automated as far as is possible in order to speed up the process and support the user, a minimum number of entries need to be made. The significance of the various fields in the dialogue above are described briefly below:

Document This box contains the name of the document to be signed together with its revision number. This is entered automatically following selection of the report and the signature icon in the previous *Report* screen.

The “Signed Rev” box is used for later reference and contains the revision number of the signed report for a given document name.

Created The *Created* information is entered automatically from the audit trail for the selected report and is based on the time of last change and the currently logged in user who made the changes.

Approval The approval and acceptance areas are selectable using the check button immediately adjacent to the respective dialogues. In order to approve a document ensure that the approval button is active. All subsequent selections will be applied then to the approval process.

Acceptance The approval and acceptance areas are selectable using the check button immediately adjacent to the respective dialogues. In order to accept a document ensure that the acceptance button is active. All subsequent selections will be applied then to the acceptance process.

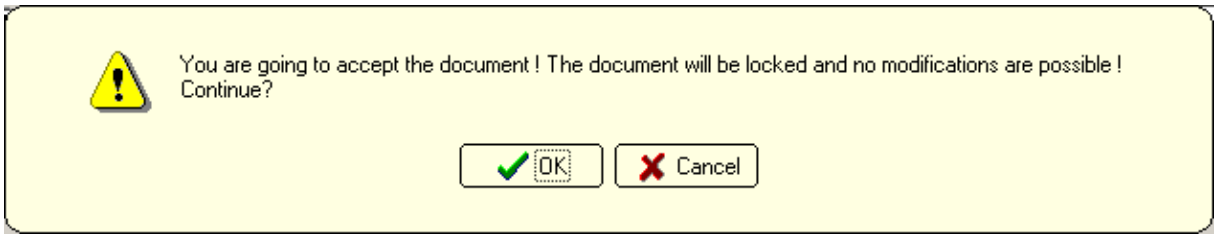
Login Name This is a drop-down selection list which allows selection of the user who is executing the signature. Only those users with the appropriate rights are displayed in the list, i.e. for acceptance only users with acceptance rights will be displayed. Select your user name from the list.

Full Name The full name is entered automatically once the user name has been selected as described above. The full name is defined initially as part of the login definitions and cannot be changed here.

Password Entry of the user password is mandatory before any signature process can be successfully concluded.

Comment Here a comment relating to the signature can be entered and this will be stored with the other signature details and also shown on all printed reports.

Once a document has been signed off and accepted it is no longer possible to change that document, therefore there are a series of prompts appearing to ensure that the user is aware of this process before actually proceeding. The final prompt appears after the signee has confirmed that the document should be signed off and is the final safety check before closing the document:



Caution *Only click on OK here if you are absolutely certain that the document in its current form is acceptable.*

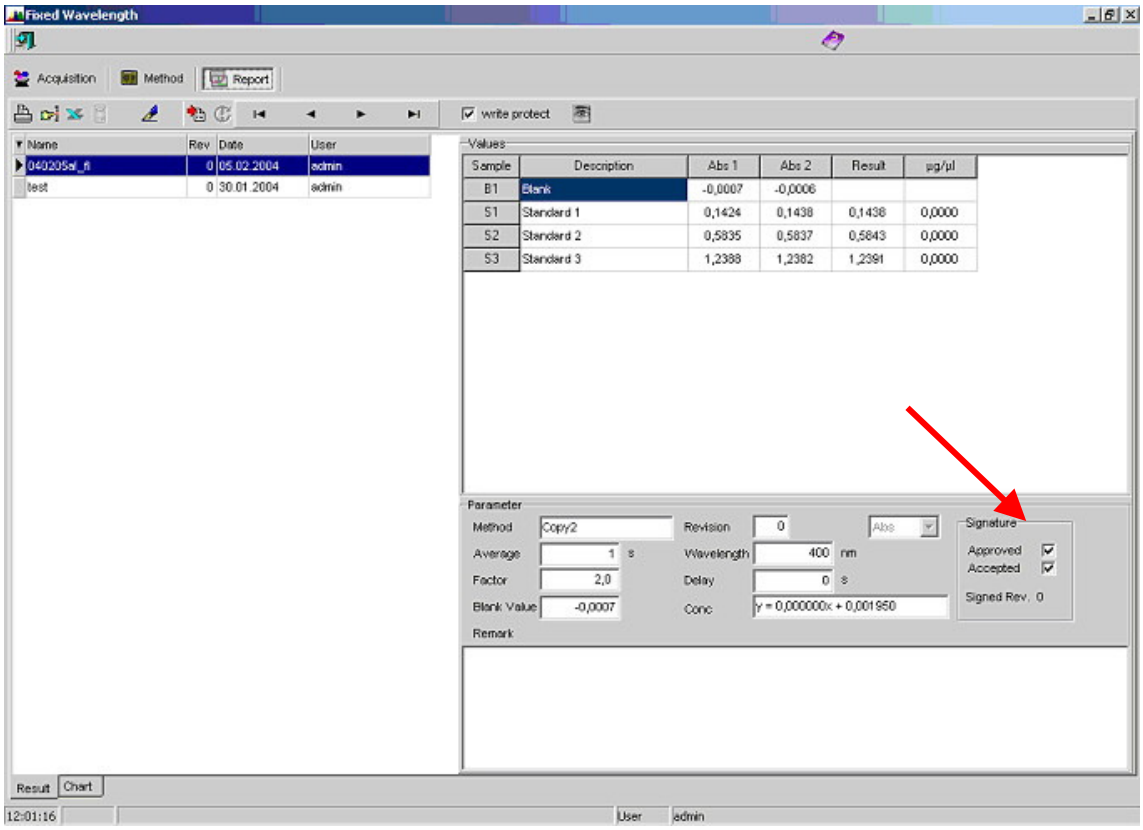
2.9.4.2. Signature Status Indications

2.9.4.2.1. Quick Overview

There are various indications to show the status of a report and whether it has in fact been signed off and accepted.

All signed reports in the list are shown with a shaded background so that the user can immediately identify those reports in the list which have been signed and accepted.

The status of a signed report in the report list is shown automatically when the report is selected in the report list:

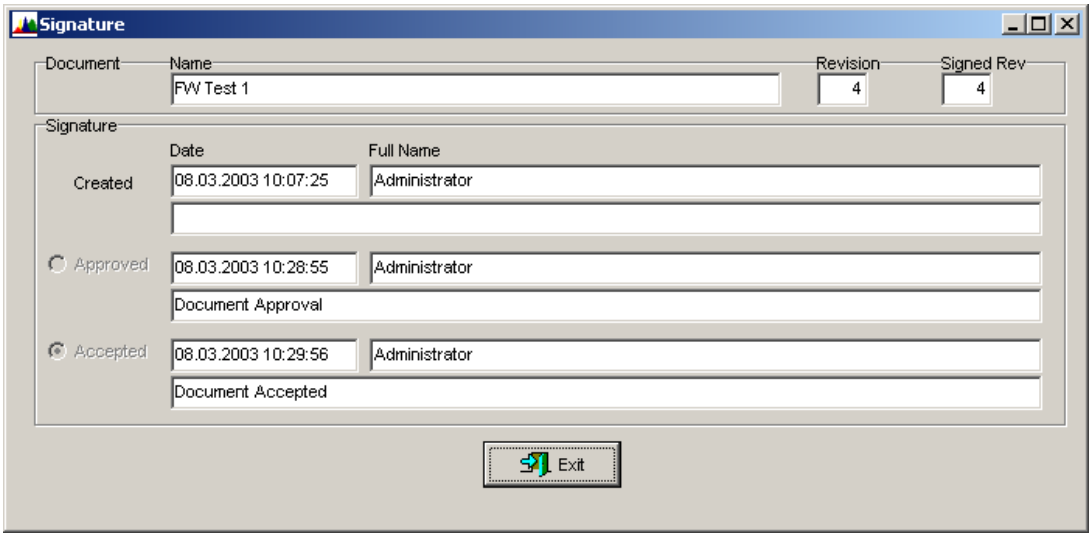


The *Approval* and *Accepted* checkboxes are only checked for a signed report. The *Signed Rev* field always carries the revision number of the signed report, if there is no entry in this field then no signed report exists for that particular named report.

It is also possible to partially sign a report, e.g. only approval, and in this case only the *Approval* box would be checked.

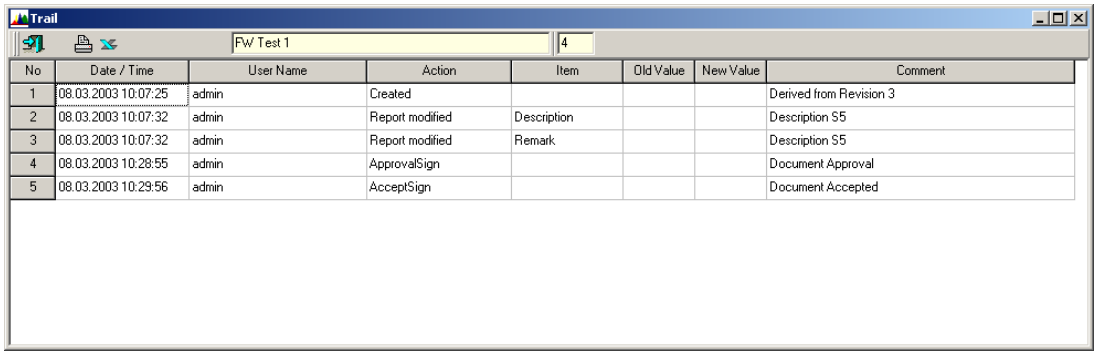
2.9.4.2.2. Detail Overview

By clicking on the *Signature* icon it is possible to see the complete details of the signature entries for the given report. Select the report from the list and click on the icon to obtain the *Signature* information:



2.9.4.2.3. Signature Audit Trail

The signature details are also recorded as part of the audit trail process and can be viewed in the report trail:



2.9.4.3. Deleting a Signed Report

For a given report it is only possible to have one signed report with the respective report name. In rare cases it may be necessary to correct a signed report after signature and then re-sign it.

The UVS software allows a signed report to be deleted by users with administrator rights only and the deletion is recorded in a separate *Deleted Reports Audit Trail*.

A new report can be signed in the normal way as described above.

3. OPTIONS AND ACCESSORIES

3.1. AUTOMATIC CELL CHANGER

3.1.1. Installation

Switch off the instrument and plug in the cable on the accessory board connector in the sample compartment. Switch on the instrument and start the UVS software. The cell changer will be recognised by the software during the initialisation process.

Access to the cell changer is possible in all modes using either direct control in the acquisition screen for single measurements or integration into a method for automatic processing of samples. The cell changer mode can be set as described below during either of these processes..

3.1.2. Cell Changer Mode (only UVSX)

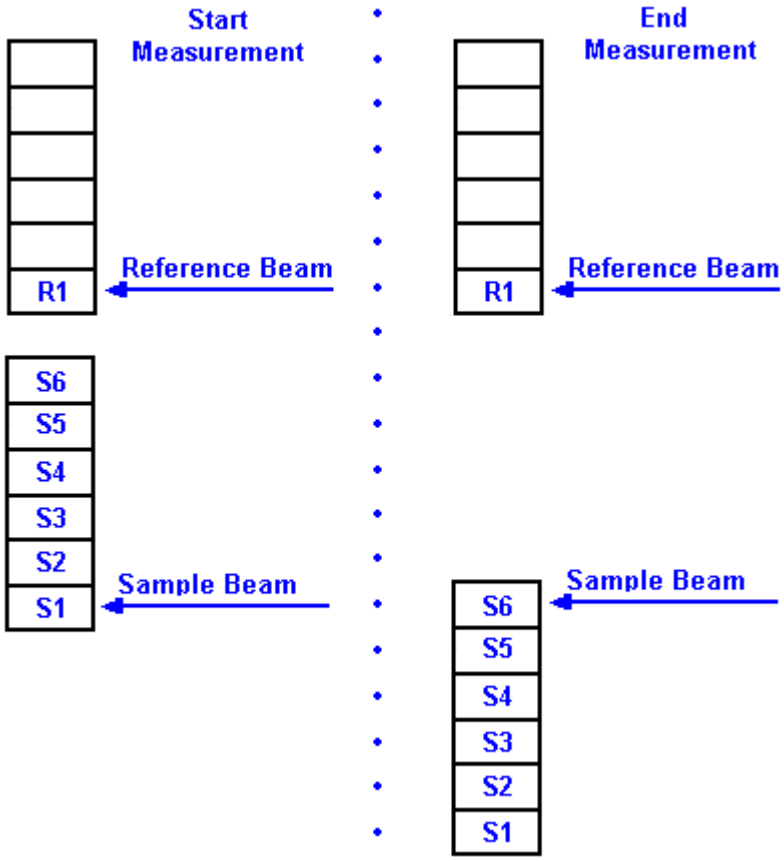
The cell changer allows three different operation modes and the mode is selectable via the *Cell Changer* dialogue in, for example, the *Acquisition* screen:

Click on the drop-down menu in *Mode* to select the required mode from a list.

3.1.2.1. 6 samples / 1 reference.

This mode allows measurement of 6 samples in the sample cell holder against 1 reference in position 1 of the reference cell holder. Only the sample cell holder moves during measurement.

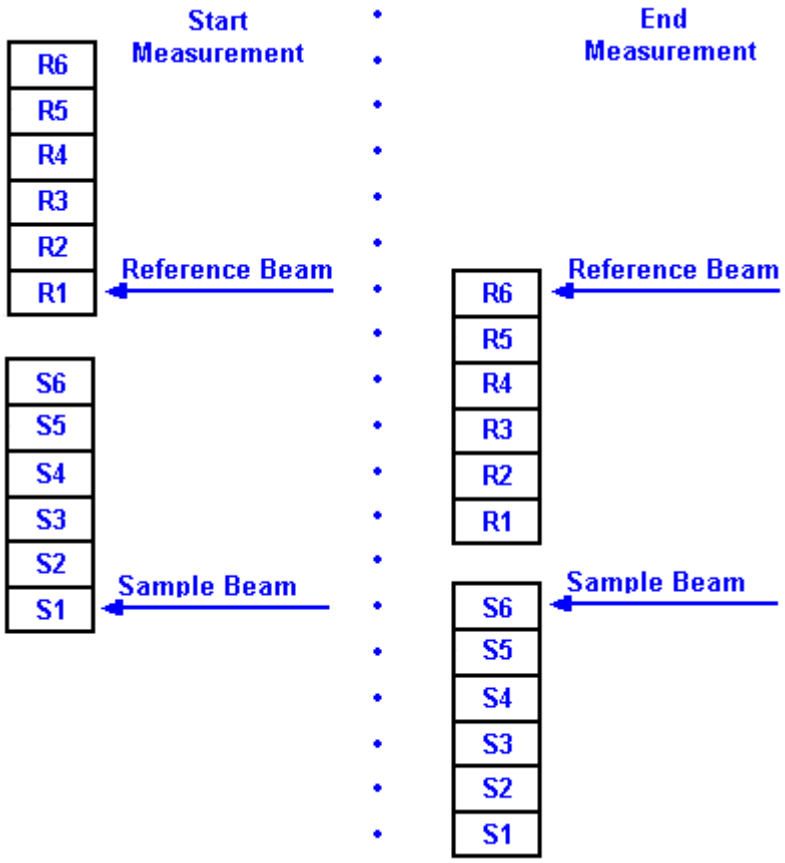
The figure below shows the cell holder positions at start and end of a measurement if all 6 cells are measured.



3.1.2.2. **6 samples / 6 references.**

This mode allows measurement of 6 samples in the sample cell holder against 6 references in the reference cell holder. Both holders move simultaneously during measurement.

The figure below shows the cell holder positions at start and end of a measurement if all 6 cells are measured.

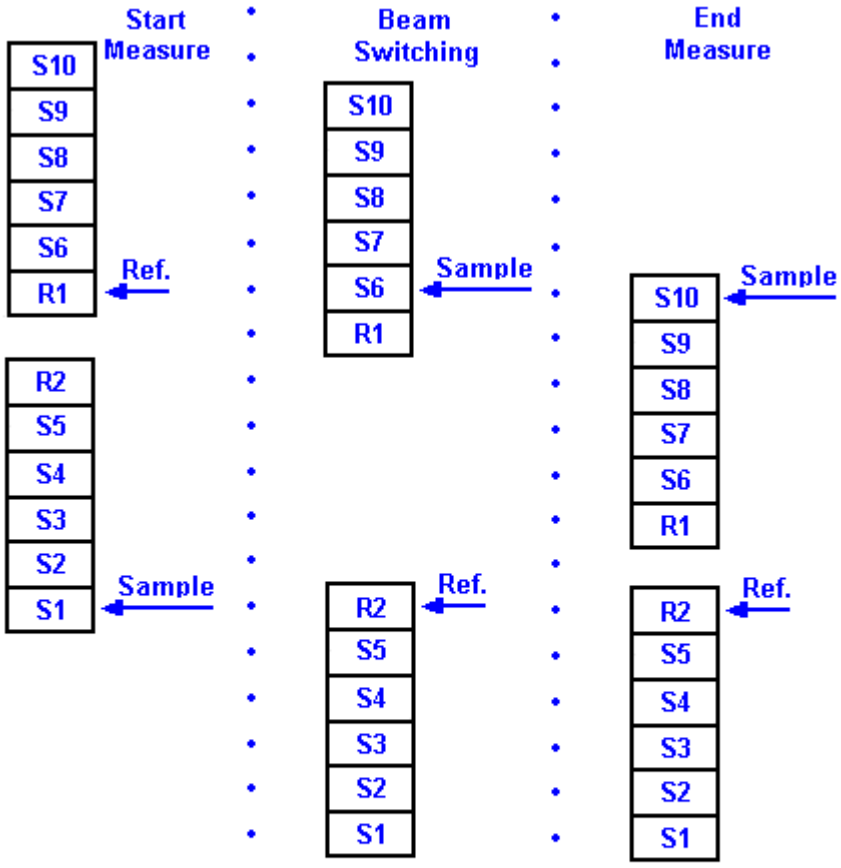


3.1.2.3. **10 samples / 2 references.**

This mode allows measurement of 10 samples (5 in the sample cell holder and 5 in the reference cell holder) against 2 references:

- Ref. 1 in position 1 of the ref. cell holder
- Ref. 2 in position 6 of the sample cell holder

Both holders move independently during measurement:

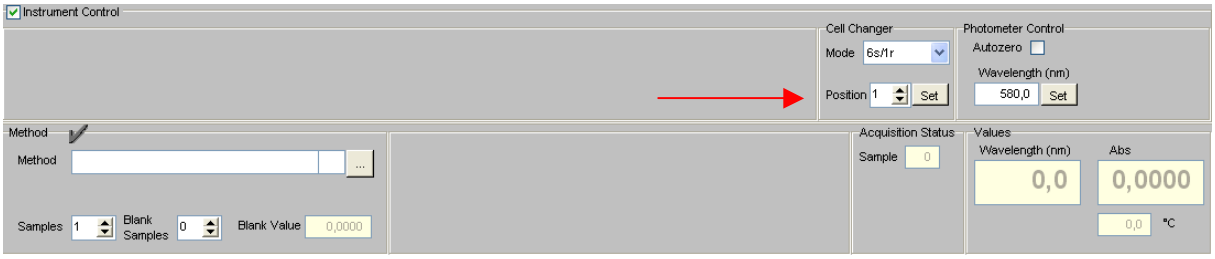


If more than 5 samples are selected in the 10 samples against 2 references mode the sample and reference beams are exchanged after the fifth sample has been measured. This unique 'beam switching' is possible due to the fact that both beams have a fully symmetric optical layout combined with symmetrical data acquisition electronics.

3.1.2.4. Manual operation (only UVSX)

The cell changer can be moved manually using the *Position* spinbox in the *Acquisition* screen. The sample position will be set automatically depending on the mode setting (see above).

Select the required sample position and the press the *Set* button, the cell changer will then move to the required position for measurement.



3.1.3. Cell Changer operation in the different system methods

3.1.3.1. Auto rate assay

In this method the instrument can measure up to ten samples simultaneously when the cell changer is in use. Measurement starts with the first reading on sample 1. The cell changer then moves to the next position and measures the first reading on sample 2. This process continues until all selected samples (parameter No. OF SAMPLES) have been measured once. The instrument will then continue measurement with the second reading on sample 1 and all other samples. The whole process is repeated until the selected number of readings has been measured. Up to ten curves (depending on the selected number of samples) can be displayed on the screen during measurement.

3.1.3.2. Fixed Wavelength

Measurement starts with the first sample. After the selected *Averaging Time* the cell changer will move to the second sample. Only one reading per sample is measured and displayed. The cell changer can also be used to measure standards in *Calibration* mode.

3.1.3.3. Wavelength Scan

The complete scan is carried out on the first sample before the cell changer moves to the second position and measurement of sample 2 is carried out. This process continues until the selected No. of samples has been measured.

3.1.3.4. Time Drive

The complete Time Drive is carried out on the first sample before the cell changer moves to the second position and measurement of sample 2 is carried out. This process continues until the selected No. of samples has been measured.

3.1.3.5. Wavelength Program

All samples are measured at the first wavelength, then the wavelength is changed to the second one and all samples are measured again. This process will be repeated until all wavelengths for all samples have been measured.

3.2. Maintenance

3.2.1. Service

Only available in UVS900 version.

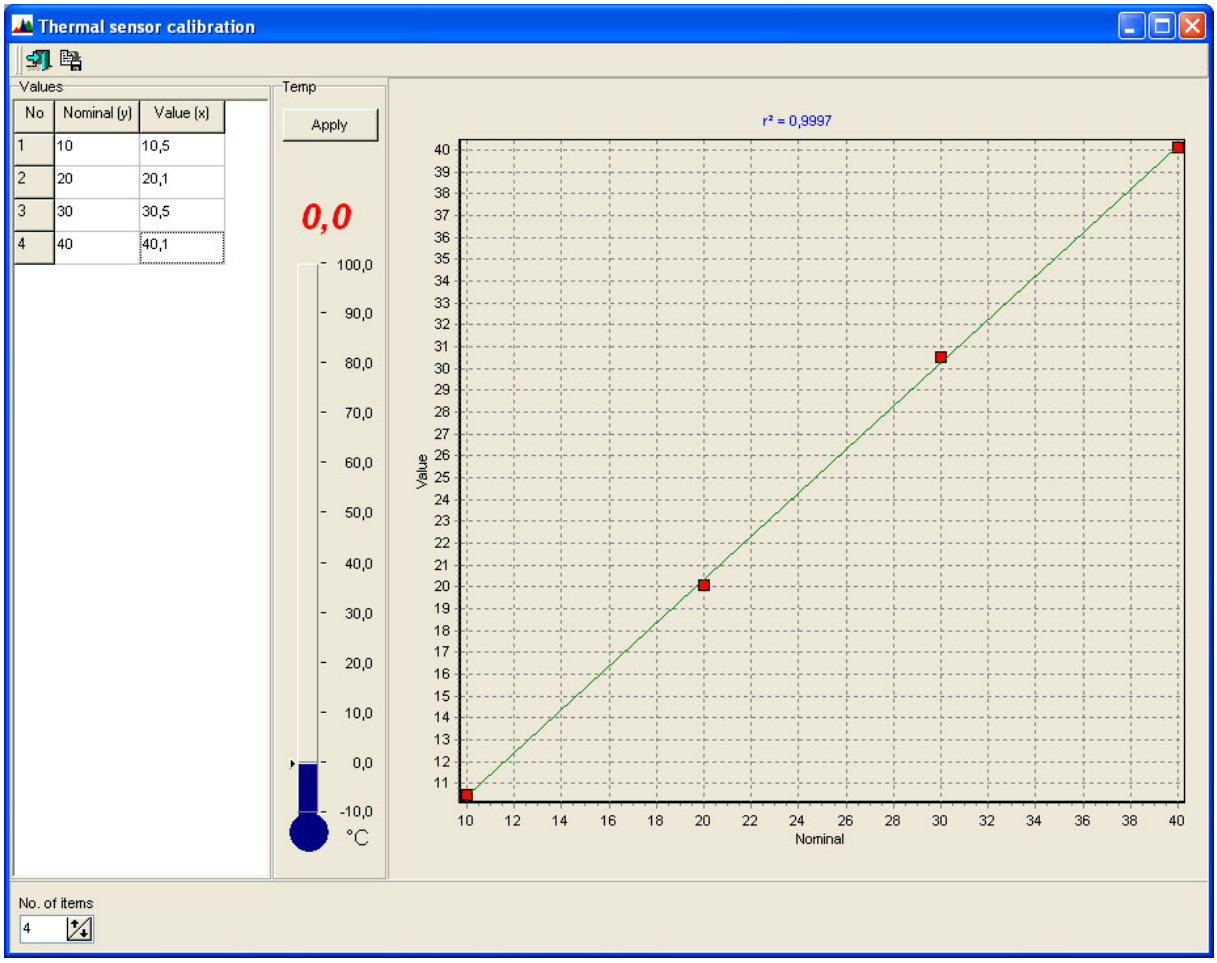
This is a service function for checking the optical system.

3.2.2. Thermal sensor calibration

Define here the calibration curve if a thermo sensor is installed. If not please let all cells blank.

Set a number of nominal values and verify your thermo sensor with a calibrated thermometer.

Example : Let your temperature goto 30 °C, press Apply and fill the correct temperature of the thermometer into the nominal value. Repeat this for 4 or 5 other temperatures and save it. Now your thermo sensor is calibrated via the curve against the nominal values of the calibrated thermometer.



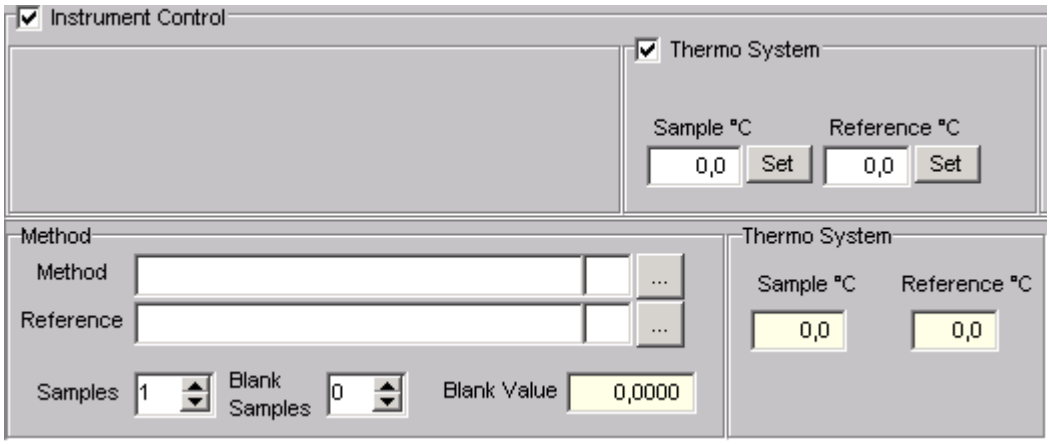
3.3. Thermosystem / Thermopack

3.3.1. Installation

Connect the thermosystem or thermopack the serial line COM 1. Start the UVS Software, the thermosystem / thermopack will be detected.

3.3.1.1. Manual operation

If the thermosystem / thermopack is detected an additional window is shown in the control/display area of the acquisition window.



Enter the required sample or reference value and the press the *Set* button, the thermosystem / thermopack will then move to the required temperature value.

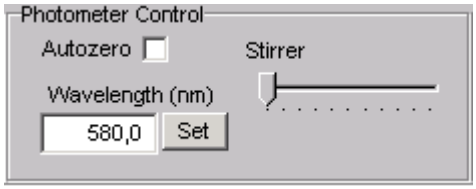
If a thermopack is detected only the sample is shown.

3.4. Stirrer (only UVSX)

3.4.1. Installation

Switch off the instrument and plug in the cable on the accessory board connector in the sample compartment. Switch on the instrument and start the UVS software. The stirrer will be recognised by the software during the initialisation process.

Access to the stirrer is possible in all modes using either direct control in the acquisition screen.

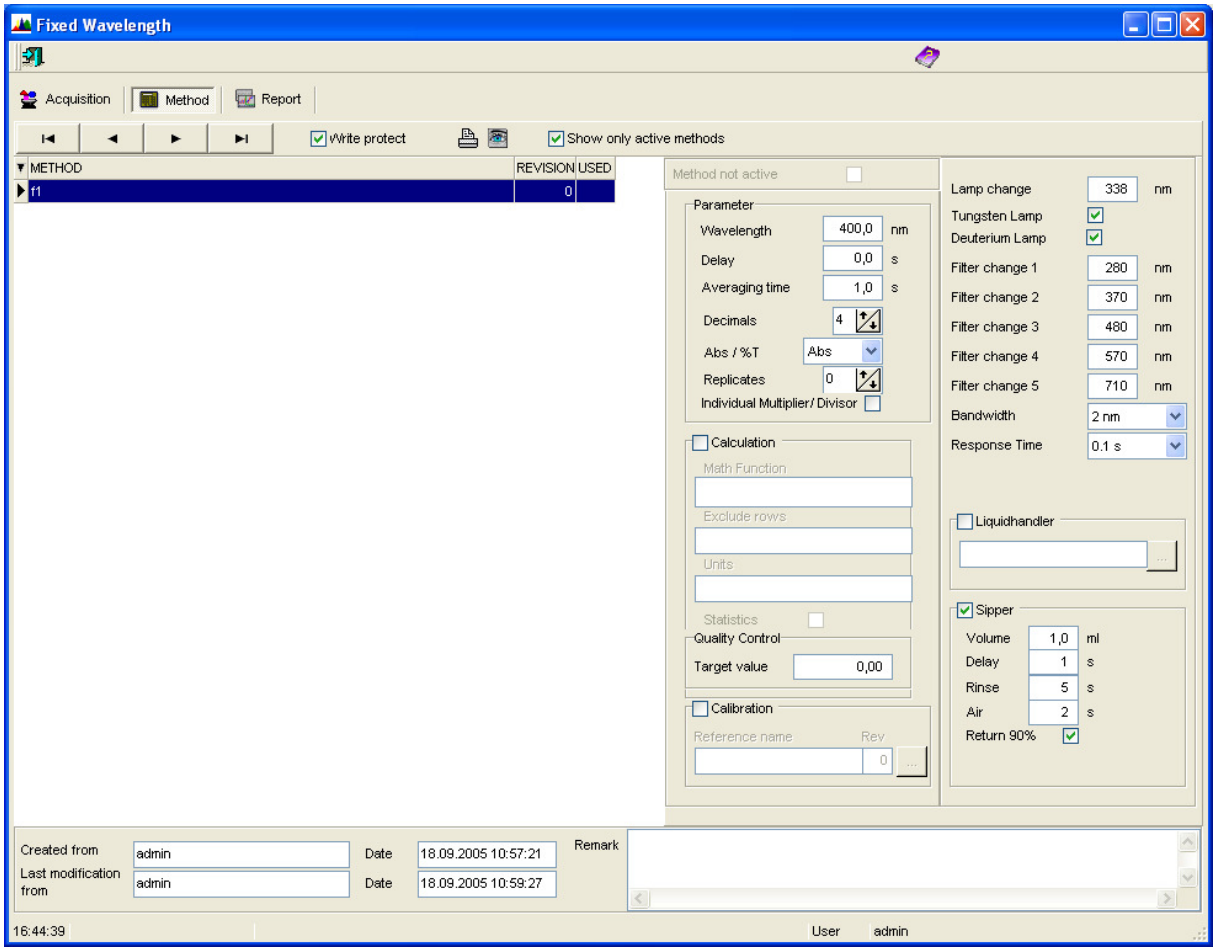


Move the track bar to set the stirrer speed, the stirrer will follow immediately.

3.5. Sipper

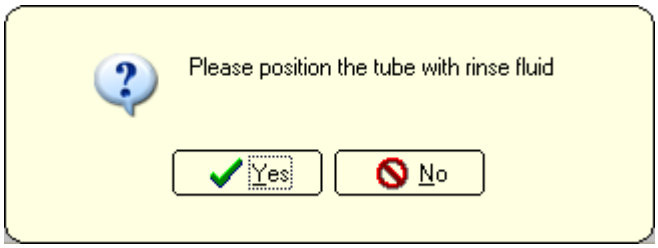
In the Method screen you can define the way for sipper handling

In addition to the volume and delay parameter the **Rinse**, **Air** and **Return 90%** was added.



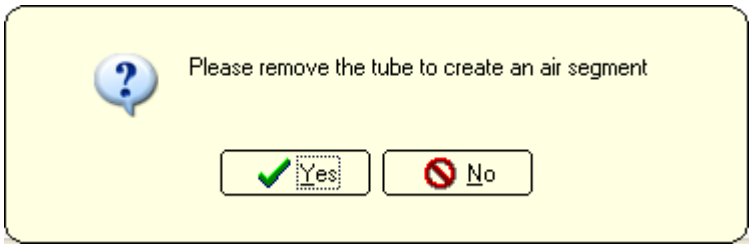
After aqcuisition the system returns 90% if activated in the method.

Then ask the system ask for rinsing (if the rinse value > 0)



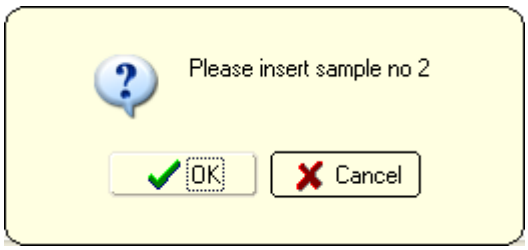
After confirming (you can use mouse or press ENTER or BLANK for yes, ESCAPE for no) rinsing starts with the rinsing time.

After this the system ask for removing the tube for air segment (if the air value > 0)



After confirming (you can use mouse or press ENTER or BLANK for yes, ESCAPE for no) rinsing starts with the air time.

Next Sample:

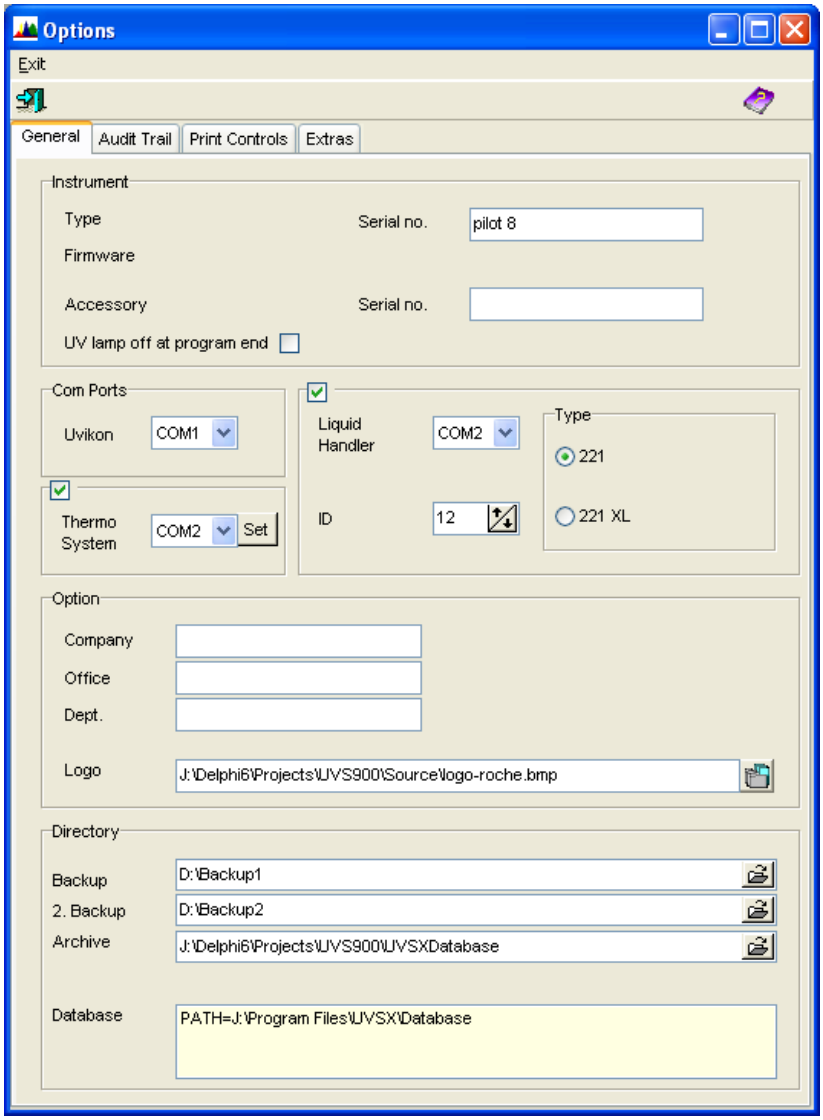


3.6. Liquid handler

The gilson liquid handler (221,221XL) can be controlled by the software if the module is installed.

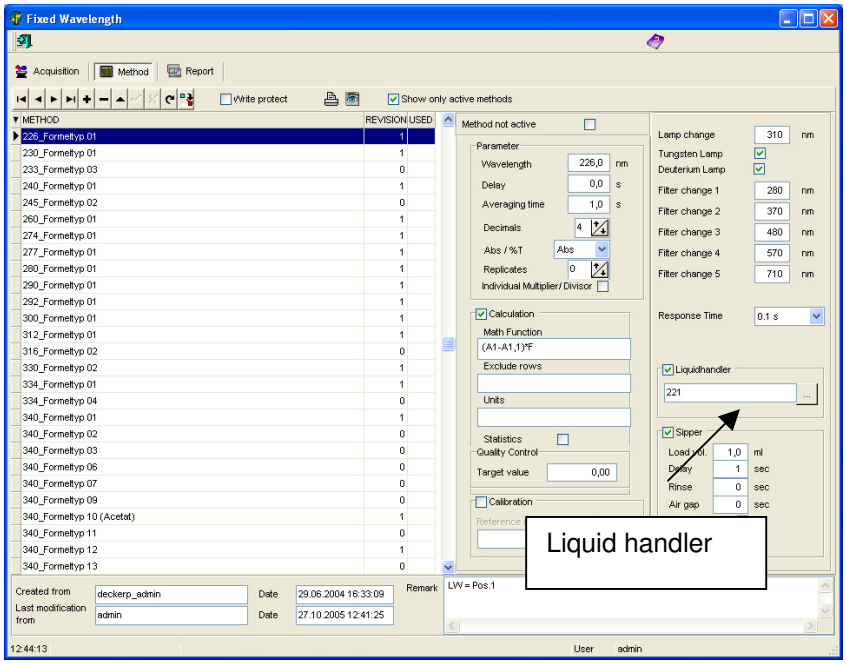
Prepare operation of liquid handler:

Activate in options menu the liquid handler by ticking the checkbox. Select the serial port connected to the liquid handler. Please check that this port is free and the baudrate of the 221 is set to 9600.
Select the type of the handler and the id.

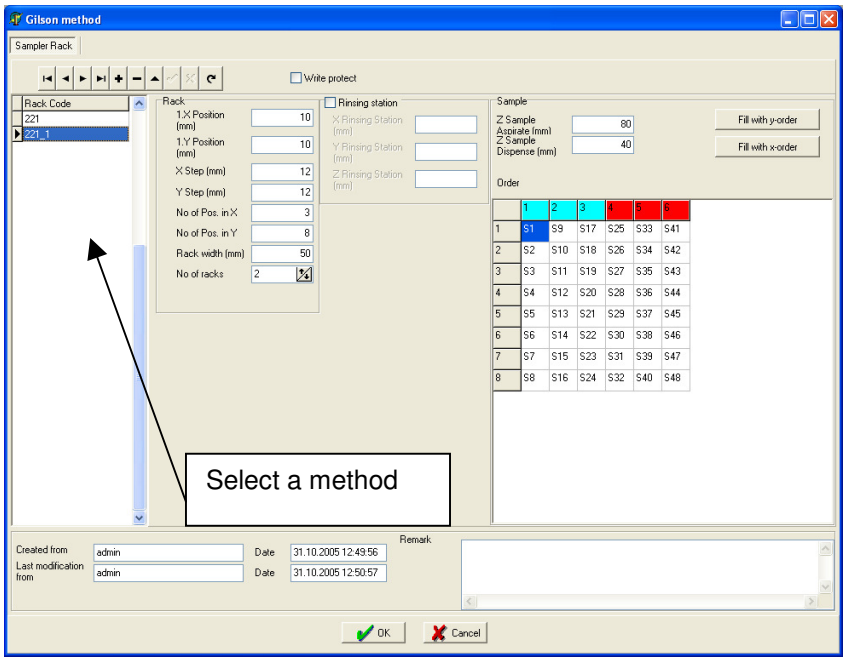


Prepare method with liquid handler :

Activate the liquid handler in the method by ticking the checkbox.
If you want to add a new liquid handler method or link this method with a liquid handler method press the button right of the box .

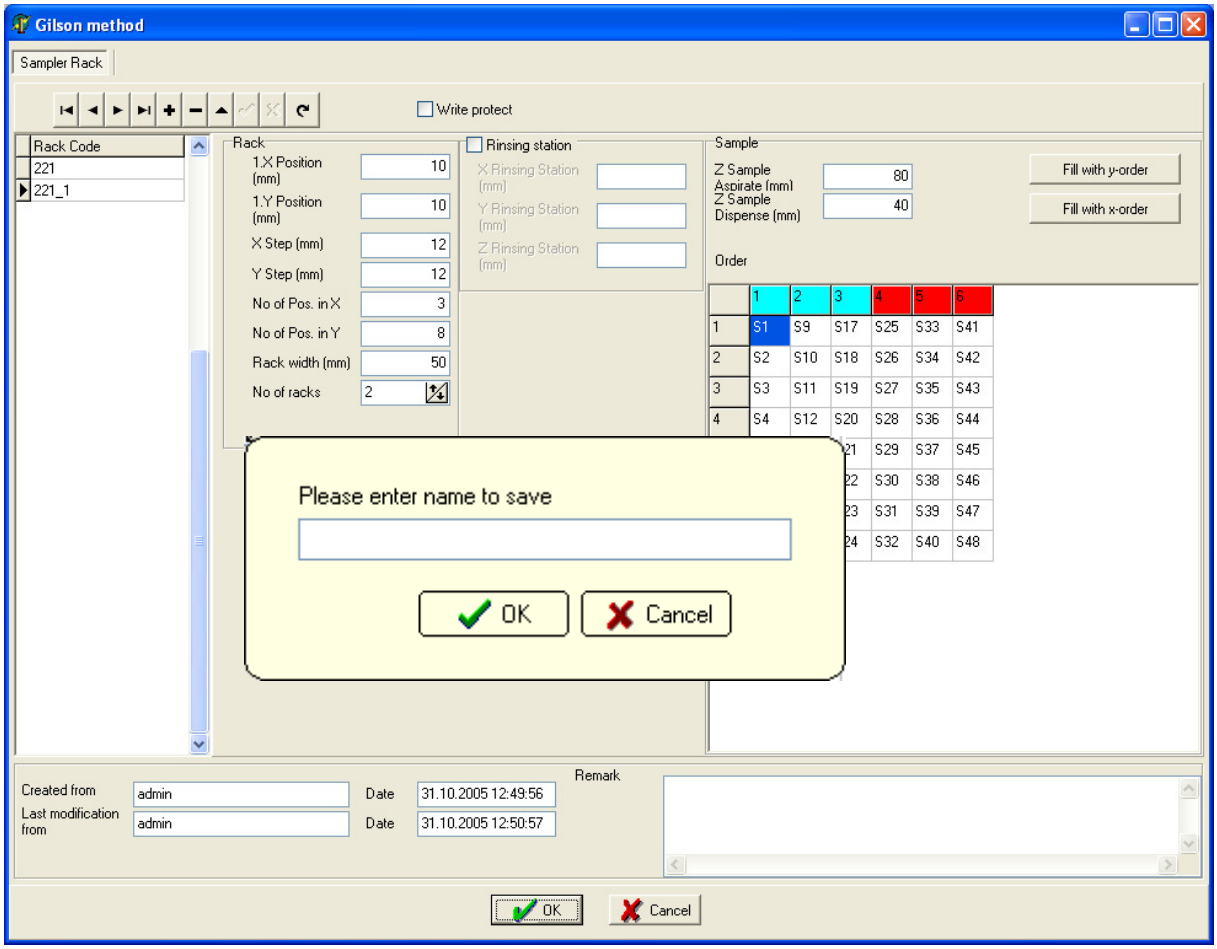


For linking with a liquid handler method select the method and press ok.



Create a new gilson method :

Press the '+' button and fill the save name in the window.



Fill the parameter as decribed below:

1. X Position : This is the first vial position in the upper left corner of the rack regarding the the zero point position of the needle in x-direction.

1. Y Position : This is the first vial position in the upper left corner of the rack regarding the the zero point position of the needle in y-direction.

X Step Distance between 2 adjacent vial position in x direction
Y Step Distance between 2 adjacent vial position in y direction

No of Pos in X Number of positions per rack in x direction
No of Pos in Y Number of positions per rack in y direction

Rack width Width of a rack in mm

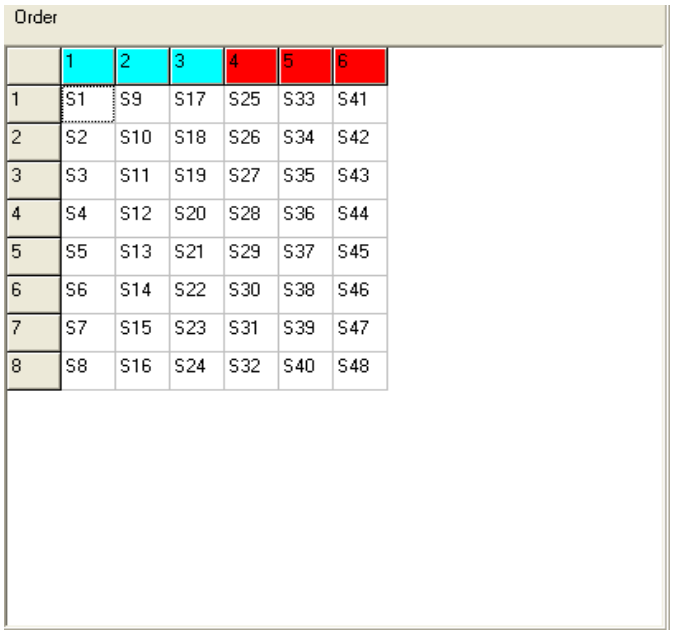
No of racks Total count of racks on the liquid handler

If you have a rinsing tube on the liquid handler, please fill the position of this tube in the rinsing station section.

How to prepare the sample positions :

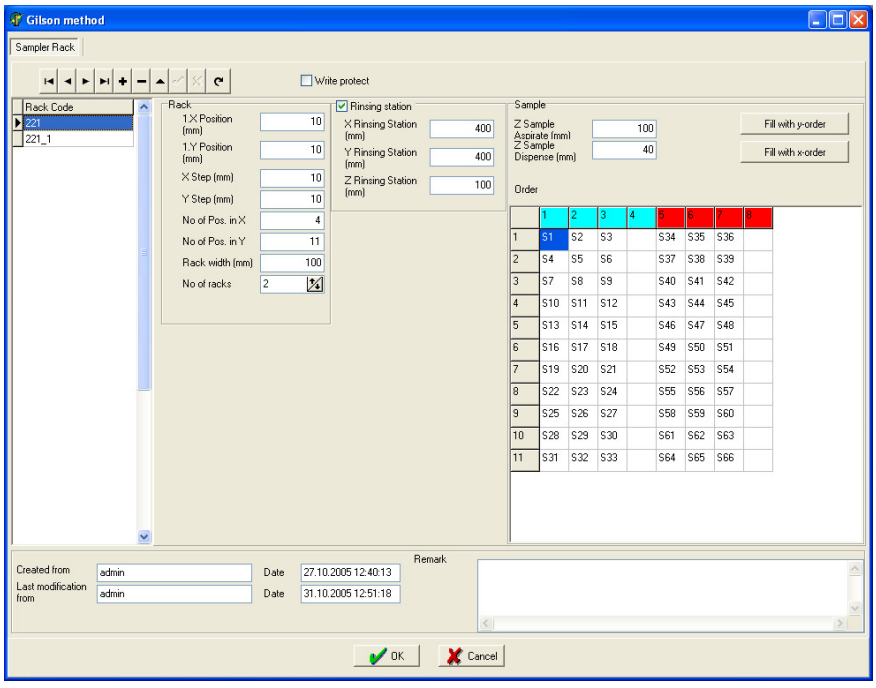
The sample position in the racks for acquisition must have the exact the same order as defined here. Please check the positions before you start the acuisition otherwise the system get the wrong sample.

In this example the sample positions are filled with y-order.



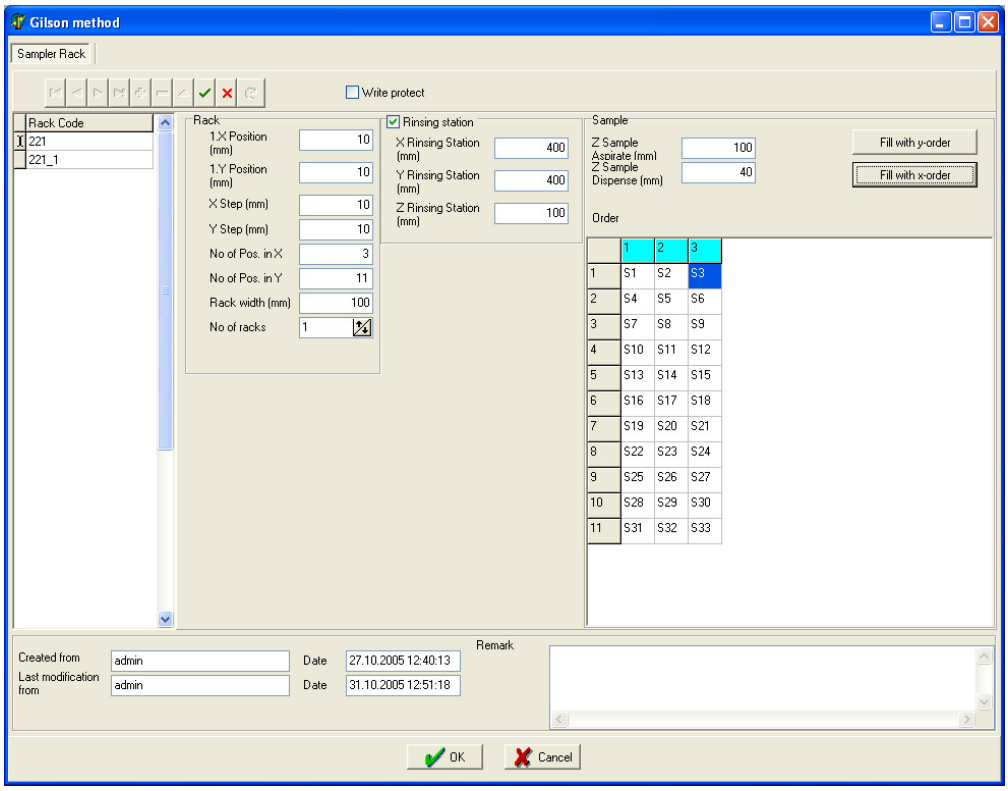
	1	2	3	4	5	6
1	S1	S9	S17	S25	S33	S41
2	S2	S10	S18	S26	S34	S42
3	S3	S11	S19	S27	S35	S43
4	S4	S12	S20	S28	S36	S44
5	S5	S13	S21	S29	S37	S45
6	S6	S14	S22	S30	S38	S46
7	S7	S15	S23	S31	S39	S47
8	S8	S16	S24	S32	S40	S48

Example of a sample with 2 replicates in a rack with 4 columns. The 4th column is free.

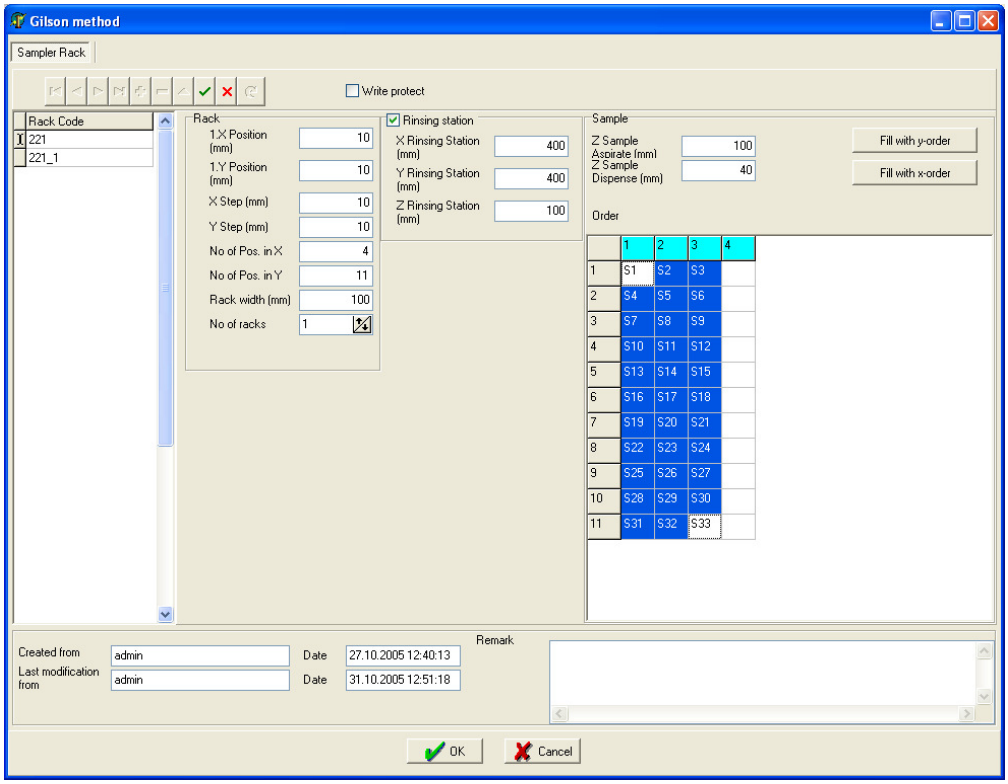


How to use it :

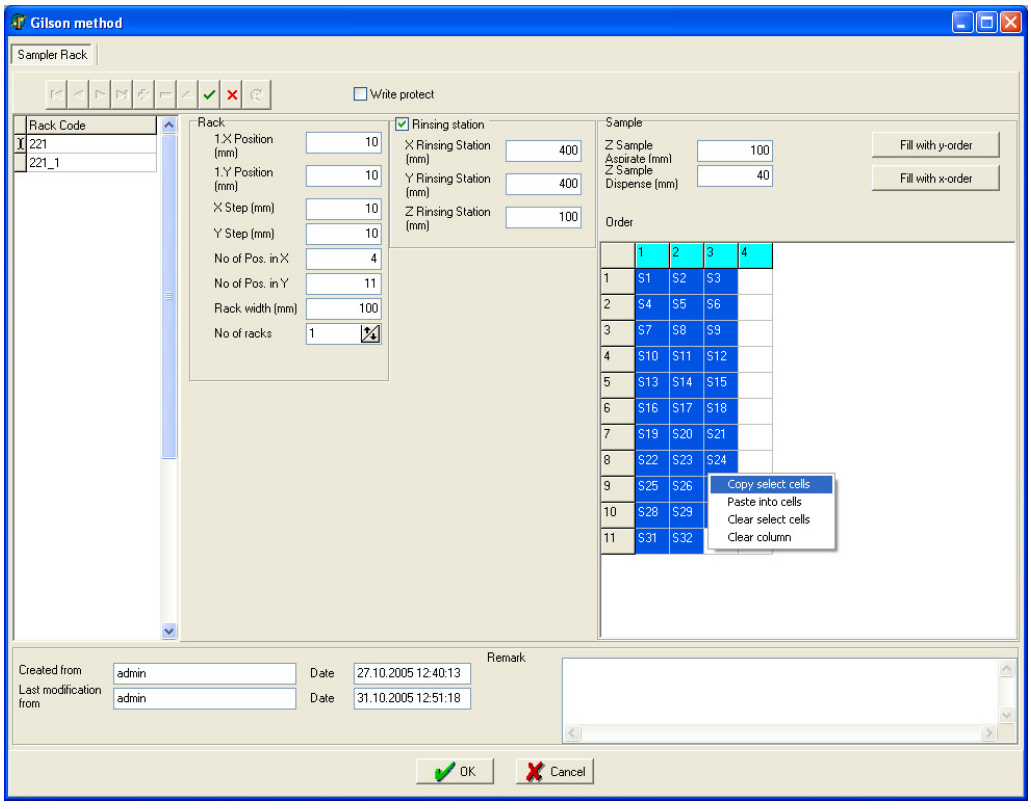
Create a method with 3 'No of pos in x' and fill with x -order



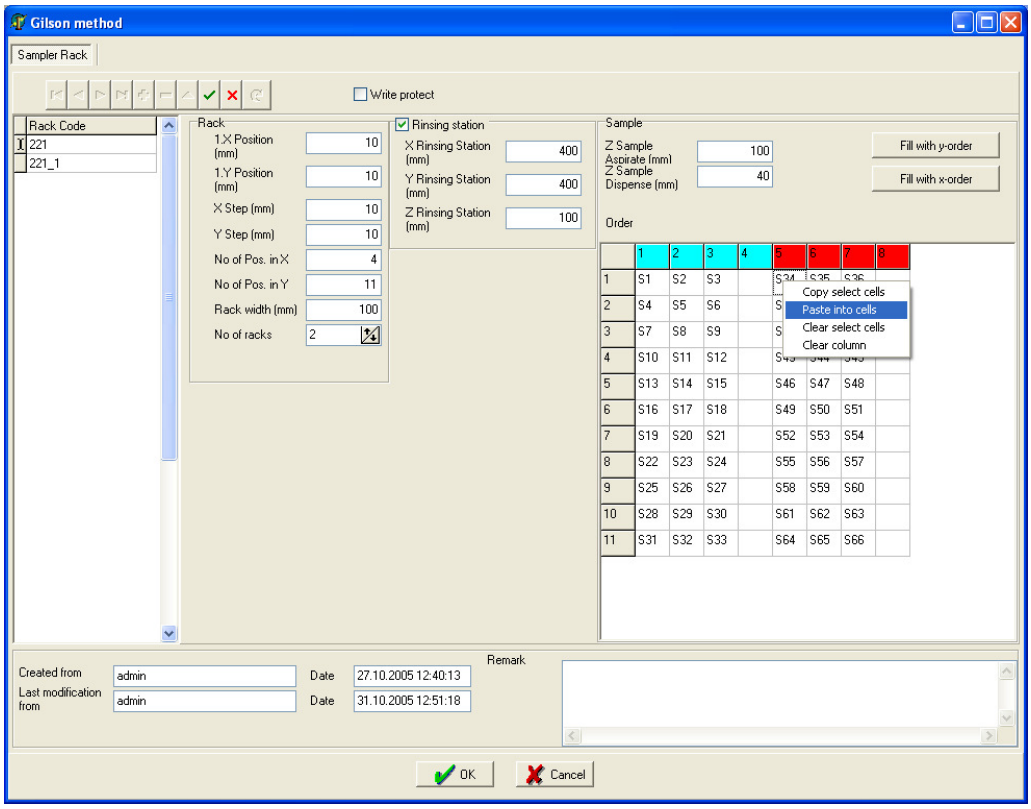
Set 'No of pos in x' to 4 positions and select an area of positions by pressing shift and left mouse button on position 1-1. Then move to position 3-11 with holding down shift and left mouse button and release the mouse button at the position 3-11. The selected area is marked as blue except the first and the last position.



Copy the selected cells by pressing the right mouse button.



Set No of racks to 2, goto position 5-1 and paste the prior selected cells.



Note : The number of samples must be equal or higher than the number of samples of the acquisitions, otherwise the handler is not able to find any position.

Save the method with the post button

3.7. Katalase

Katalase is a module for calculation a time by a given absorbance start and end point in time drive if the module is installed.

A decreasing reaction will acquire in timedrive. If the absorption has reached two defined points, the time between is calculated.

The parameters must be entered in the ‚Edit Calculation Parameter'.

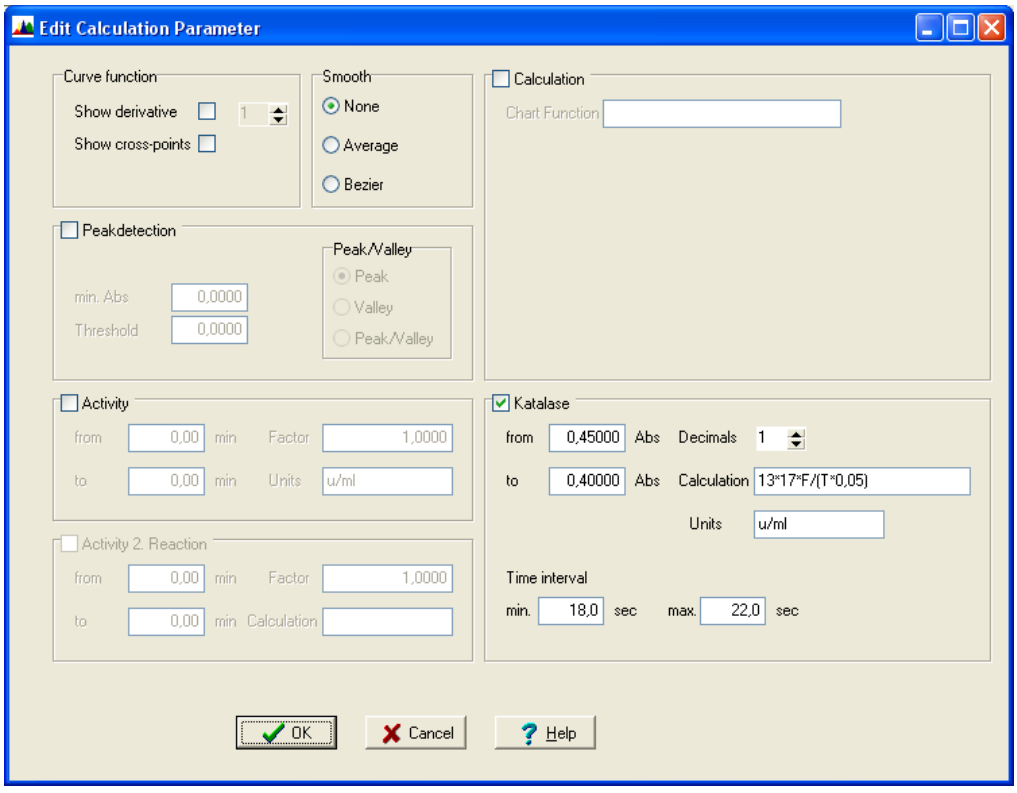
Checkbox Katalase should be activated, Aktivity must be not activated.

From : Absorbance value for start point.
To : Absorbance value for end point.
Decimals : Decimal points of the result
Calculation: Calulation formula
Possible variables : F – individual factor per sample
T – calculated time from start to end point.

Example : 13*17*F/(T*0,05)

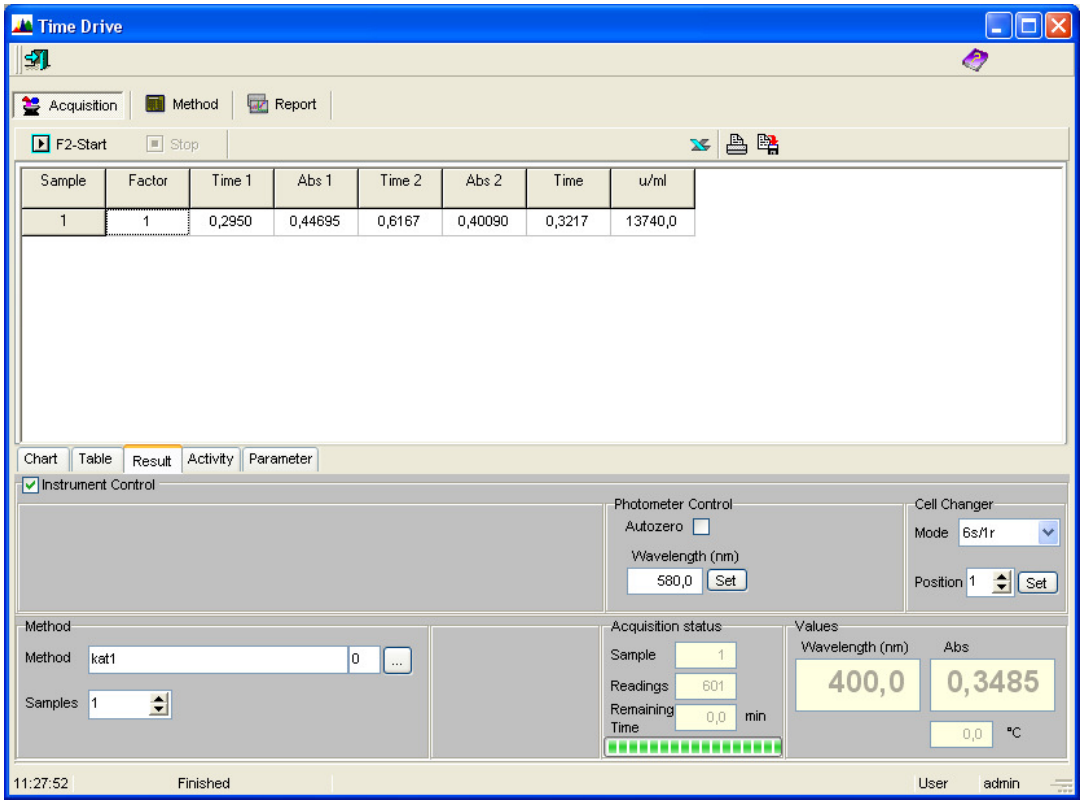
Time Interval: The result will be marked with * if the calculated time is outside.

Units: Remark of the unit.



The results are shown in the result tab sheet.

A factor per sample can be entered, if the field is blanked a value of 1 will be calulated.



The linear regression curve is shown.